ASMS

June1 - 12

REBOOT

2020

68th ASMS Conference on Mass Spectrometry and Allied Topics

The conference was presented virtually over two weeks, June 1-12, 2020. This program book contains the following sections:

- ASMS Board of Directors
- Program Acknowledgements
- Interest Groups and Committees
- Program Highlights-Special Lectures (Award, Plenary, and Tutorial)
- Awards
- Corporate Members
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- Posters
- Workshops
- Author Index

For detail on the ASMS Meeting presented by the Board of Directors, please see the Conference Proceeding for 2020 and the document folder entitled 'ASMS Meeting.'

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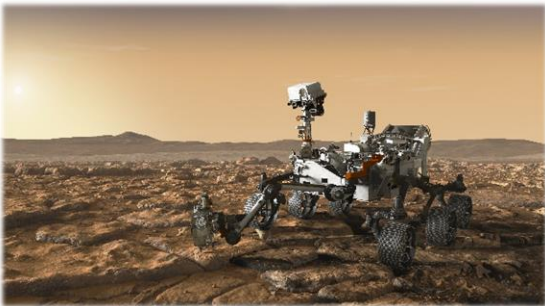Christopher Rose
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Award, Plenary, and Tutorial Lectures

Recordings of lectures listed below are available to members at
ASMS.org > Publications > Award, Plenary, and Tutorial Lectures page.

Tutorial Lecture
Peter Nemes (University of Maryland, College Park)
Single Cell Mass Spectrometry

Tutorial Lecture
Heather Desaire (University of Kansas)
Glycoprotein Analysis for Understanding Human Disease

Special Lecture
Corinne Moss-Racusin (Skidmore College)
Is There Still Gender Bias in Academic Science (and Does It Matter)? What the Scientific Studies Say

Opening Plenary
Patricia M. Beauchamp (California Institute of Technology)
Mars 2020

|	
	Award Lecture: John B. Fenn Distinguished Contribution in Mass Spectrometry Michael L. Gross (Washington University at St Louis) *Also see awards announcement on following pages.*
	Award Lecture: Biemann Medal Ying Ge (University of Wisconsin-Madison) *Also see awards announcement on following pages.*
	Closing Plenary Stephen Brusatte, University of Edinburgh New Dinosaur Discoveries

ASMS AWARDS

American Society for Mass Spectrometry is pleased to announce 2020 Awards.
For more details please contact info@asms.org.

JOHN B. FENN DISTINGUISHED CONTRIBUTION AWARD
2020 Recipient: Michael L. Gross

The ASMS Award for Distinguished Contribution in Mass Spectrometry honors the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray Ionization. John joined ASMS in 1986 and remained an active member until his passing in 2010. The award is conferred at the ASMS Annual Conference with the presentation of a $10,000 cash award, a recognition plaque, and the award lecture.
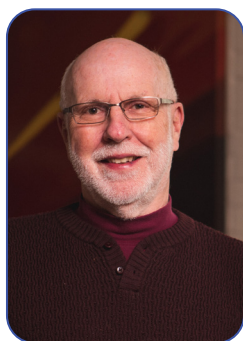
Dr. Michael L. Gross is the recipient of the 2020 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry, for innovative and integrative MS-based footprinting for structural proteomics. The development of Fast Photochemical Oxidation of Proteins (FPOP), whereby covalent modifications of proteins can occur with hydroxyl radicals on the microsecond time scale, enables the study of protein conformation, folding, aggregation, and the identification of extracellular domains.

Additionally, Dr. Gross combined MS with hydrogen-deuterium exchange (HDX) as a complement to FPOP for the determination of protein affinity, and he has developed protein chemistry methods for glycine ethyl ester (GEE) footprinting of side chains of aspartate and glutamate. Implementing these methods in combination has allowed significant insights to be gained with regard to many proteins with important therapeutic and clinical implications. His integrative approach is setting the standard for structural proteomics, as evidenced by its wide application in the pharmaceutical industry for the characterization of therapeutic proteins.

Dr. Gross is Professor of Chemistry and of Immunology and Internal Medicine (School of Medicine), Washington University in St. Louis.

AL YERGEY MS SCIENTIST AWARD
2020 Recipient: Rachel Ogorzalek Loo

The Al Yergey Mass Spectrometry Scientist Award is sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes. This award is named in memory of Al Yergey a well-respected scientist who was known as a dedicated mentor.

Dr. Rachel Ogorzalek Loo is the 2020 recipient of the Al Yergey MS Scientist Award. She has been involved with mass spectrometry for nearly thirty years, currently serving as a Research Biological Chemist at UCLA. She has co-authored over 125 peer-reviewed scientific papers and has significantly contributed to our understanding of electrospray ionization, charging, and protein structure. Dr. Loo was one of the first to pursue the idea that ESI charge state distributions depend on protein solution phase structures. She continues to explore the fundamental aspects of ESI, proposing new mechanisms in a Critical Insights article for JASMS in 2014.

Dr. Loo has also served as a mentor to countless graduate students, postdocs and scientists and given her time to serve the mass spectrometry and greater scientific community at large.

RON HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN *JASMS*
2020 Recipient: Stephen J. Valentine

The Ron Hites Award recognizes an outstanding publication of original research based on innovative aspects, technical and presentation quality, and likely stimulation of future research or applications. The award is named to honor Professor Ron Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS. The award includes $2,000 and certificates.

The 2020 Ron Hites Award recognizes **Dr. Stephen Valentine**, West Virginia University and co-authors for their paper Comprehensive Peptide Ion Structure Studies Using Ion Mobility Techniques: Part 3. Relating Solution-Phase to Gas-Phase Structures; Samaneh Ghassabi Kondalaji,Mahdiar Khakinejad, Stephen J. Valentine; *J. Am. Soc. Mass Spectrom*. (2018) 29:1665-1677.

ASMS AWARDS

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For more details please contact info@asms.org.

BIEMANN MEDAL
2020 Recipient: Ying Ge

The Biemann Medal is awarded to an individual early in his or her career to recognize significant achievement in basic or applied mass spectrometry. The Medal is conferred at the ASMS Annual Conference with the presentation of a $5,000 cash award, a recognition plaque, and the award lecture.

Dr. Ying Ge iis the recipient of the 2020 Biemann Medal for significant contributions to high-resolution mass spectrometry (MS)-based top-down proteomics and their application to cardiac diseases. Dr. Ge has demonstrated that Fourier transform ion cyclotron resonance (FT-ICR) MS with electron capture dissociation (ECD) is especially useful for mapping labile post-translational modifications, and she has isotopically resolved large proteins with high mass accuracy, allowing the characterization of very large proteins directly from human heart tissues.

To address the many challenges in top-down proteomics, she has successfully developed novel strategies for protein extraction, solubility, and separation to enable comprehensive top-down MS characterization of biologically critical cardiac proteins. Her technical excellence has allowed her to make important discoveries in myofilament biology and gain novel insights into the understanding of cardiac diseases. For example, she has identified phosphorylation of cardiac troponin I and actin isoform switching as potential biomarkers for chronic heart failure by top-down MS. Dr. Ge's significant contributions to both MS-based top-down proteomics and her fundamental insights into cardiac pathologies make her an outstanding recipient of the Biemann Medal.

Dr. Ge is Professor of Cell and Regenerative Biology and Chemistry at the University of Wisconsin at Madison.

RESEARCH AWARDS

Research awards promote the research of academic scientists within the first four years of joining the tenure track or research faculty of a North American University at the time the award is conferred. The awards, in the amount of $35,000 are fully supported by Bruker, Thermo Fisher Scientific, and Waters Corporation.

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2020 Recipient
Ian K. Webb
Indiana University

RESEARCH AT PRIMARILY UNDERGRADUATE INSTITUTION (PUI) RESEARCH AWARD
2020 RECIPIENT: CHRISTINE HUGHEY SPONSORED BY AGILENT TECHNOLOGIES

This award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The award of $20,000 is made to the recipient's institution on behalf of the recipient's research.

2020 Recipient
Christine Hughey
James Madison University

2020 POSTDOCTORAL CAREER DEVELOPMENT AWARDS

Postdoctoral Career Development Awards in the amount of $5,000 promote the professional career development of postdoctoral fellows in the field of mass spectrometry.

2020 Recipient
Juan Aristizabal Henao
University of Florida

2020 Recipient
Wout Bittremieux
University of California -San Diego

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2020 Recipient
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ORALS

REBOOT

All orals will be a part of the on-demand content for the ASMS 2020 Reboot. Registrants will have access to the short abstract, ePoster, and optional poster presentation video June 1 - August 31, 2020 via the mobile app and online planner (these tools become available on June 1.)

In addition there will be a webinar 'Watch party' followed by Live Q&A with speakers in week 2 of the Reboot program (June 8-12). 'Watch party' will be viewing of the six talks (also available on-demand at any time beginning June 1.)
Registered attendees interested in only the Live Q&A will be advised to join the webinar after approximately two hours (time for six 20-minute talks to play.)

Note that some sessions have 'empty slots' listed. For these sessions chairs will seek to find alternates from among the poster presenters. We will update this Orals document as alternates for these slots are confirmed.

Thank you for your interest in the ASMS 2020 Reboot program.
More information on the Reboot may be found here. To register and have the full-access described above, please go here.

MOA am: Instrumentation: Innovations in Mass Analyzers
Chair: Chad Weisbrod (National High Magnetic Field Laboratory)

MOA am 08:30   **Coulombic interaction as a new ion ejection method for ion trap mass spectrometry analysis**; Xiaoyu Zhou[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

MOA am 08:50   **Microparticle charge detection mass spectrometry using printed circuit board arrays**; Elaura Gustafson[1]; Tabitha Caldwell[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

MOA am 09:10   **Highly Multiplexed Individual Ion Mass Spectrometry in an Orbitrap for Both Native and Top-Down MS**; Jared O. Kafader[1]; Ping F. Yip[2]; Bryan P Early[1]; Kenneth R Durbin[1]; Neil L. Kelleher[1]; Michael W. Senko[2]; Philip D. Compton[1]; *[1]Northwestern University, Evanston, IL/60208; [2]Thermo Fisher Scientific, San Jose, CA*

MOA am 09:30   **Parallel DDA and DIA acquisition of spectra in an ion cyclotron resonance array cell**; Jared P. Mohr[1]; Sung-gun Park[1]; Gordon A. Anderson[2]; James E. Bruce[1]; *[1]University of Washington, Seattle, WA; [2]GAA Custom Engineering, LLC,, Benton, WA*

MOA am 09:50   **FT mass spectrometer based on multielectrode harmonized Kingdon trap in FT ICR mode of operation**; Eugene (evgeny) Nikolaev[1, 2]; Oleg Kharybin[3]; Gleb Vladimirov[3]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation; [2]Institute of Energy Problems of Chemical Physics Russian Academy of Sc., Moscow, Russia; [3]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation*

MOA am 10:10   **A novel compact Orbitrap platform enables new applications of high-resolution accurate-mass analysis**; Jan-Peter Hauschild[1]; Amelia Peterson[1]; Erik Couzijn[1]; Eduard Denisov[1]; Denis Chernyshev[1]; Christian Thoeing[1]; Oliver Lange[1]; Bastian Reitemeier[1]; Arne Kreutzmann[1]; Wilko Balschun[1]; Aivaras Venckus[1]; Sebastian Kanngiesser[1]; Alexander Kholomeev[1]; Gregor Quiring[1]; Frank Czemper[1]; Kerstin Strupat[1]; Siegrun Mohring[1]; Tabiwang N. Arrey[1]; Julia Kraegenbring[1]; Catharina Crone[1]; Mathias Mueller[1]; Andreas Wieghaus[1]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MOB am: Ion Mobility: Structure
Chair: Tara Pukula (University of Adelaide)

MOB am 08:30   **Ion mobility spectra of fragment ions produced from native top-down sequence analysis reflect type and sequence of the fragment ions**; Christian Bleiholder[1]; Fanny C Liu[1]; Kirsten Tucker[1]; *[1]Florida State University, Tallahassee, FL*

MOB am 08:50   **Annotating Collision Induced Unfolding Pathways using Electron Capture Dissociation**; Carolina Rojas Ramirez[1]; Ruwan T. Kurulugama[2]; Valery G. Voinov[3]; John C. Fjeldsted[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Agilent Technologies, Santa Clara, CA; [3]e-MSion, Inc., Corvallis, OR*

MOB am 09:10   **Use of Ion Mobility-Mass Spectrometry (IM-MS) to Characterise the Structures of Poly(L-Lysine) Dendrimers**; Florian Benoit[1]; Richard M. England[2]; Tony W. T. Bristow[2]; Perdita E. Barran[1]; *[1]Manchester Institute of Biotechnology, The University of Manchester, Manchester, United Kingdom; [2]AstraZeneca, Macclesfield, United Kingdom*

MOB am 09:30   **FAIMS and native mass spectrometry: Analysis of intact protein assemblies and protein complexes**; Oliver J Hale[1]; Eva Illes-Toth[1]; Todd H. Mize[1]; Helen Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom*

MOB am 09:50   **High-Resolution Ion Mobility Separations of Isomeric Glycoforms with Variations on the Peptide and Glycan Levels**; Pratima Pathak[1]; Matthew A. Baird[1]; Alexandre A. Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

MOB am 10:10   **Are the structures of molecular elephants enduring or ephemeral? Results from time-dependent, tandem ion mobility**; Benjamin P Zercher[1]; Seoyeon Hong[1]; Anneclaire Wageman[1]; Matthew Bush[1]; *[1]University of Washington, Seattle, WA*

	MOC am: Plants: Systems, Biotechnology, and Natural Products

Chair: Zhongping Yao (Hong Kong Polytechnic University)

MOC am 08:30   **The many and varied responses of different varieties and species of rice to a range of external stresses**; Sara Hamzelou[1]; Fatemeh Habibpourmehraban[1]; Matthew Mckay[1]; Ardeshir Amirkhani[1]; Karthik Kamath[1]; Mehdi Mirzaei[1]; Brian J. Atwell[1]; Paul A. Haynes[1]; *[1]Macquarie University, North Ryde, Sydney, Australia*

MOC am 08:50   **Development of data-independent acquisition (DIA) peptidomics approach on analyzing peptide signaling in plants**; Yet-Ran Chen[1, 2]; Sheng-Chih Hung[1, 2]; Wei-Hung Chang[1]; Ying-Lan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan; [2]National Taiwan University, Taipei, Taiwan*

MOC am 09:10   **Identification of antimicrobial peptides from plants**; Tessa B. Moyer[1]; Lilian R. Heil[1]; Leslie M. Hicks[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC*

MOC am 09:30   **Visualizing the distribution of strawberry plant metabolites at different maturity stages by MALDI-TOF imaging mass spectrometry**; Jin Wang[1]; Ethan Yang[2]; Pierre Chaurand[2]; Vijaya Raghavan[1]; *[1]McGill University, Sainte-Anne-de-Bellevue, QC; [2]University of Montreal, Montreal, QC*

MOC am 09:50   **Mass Spectrometry Elucidates Benzothiadiazole-Induced Immunity to a Bean Rust Fungus**; Bret Cooper; *USDA-ARS, Beltsville, MD*

MOC am 10:10   **A draft of the Arabidopsis proteome**; Julia Mergner[1]; Martin Frejno[1]; Markus List[1]; Maxim Messerer[2]; Daniel Lang[2]; Xia Chen[1]; Ajeet Chaudhary[1]; Hiromasa Shikata[3]; Philipp Cyprys[4]; Rashmi Hazarika[1]; Daniel Zolg[1]; Patroklos Samaras[1]; Tobias Schmidt[1]; Mathias Wilhelm[1]; Stefanie Sprunck[4]; Jan Baumbach[1]; Frank Johannes[1]; Klaus Mayer[2]; Kay Schneitz[1]; Claus Schwechheimer[1]; Bernhard Kuster[1]; *[1]TU Munich, Freising, Germany; [2]Heltmholtz Center, Munich, Germany; [3]Institute of Transformative Bio-Molecules, Nagoya, Japan; [4]University of Regensburg, Regensburg, Germany*

	MOD am: Informatics: Peptide and Protein Identification, Proteomics

Chair: Christine Carapito (IPHC)

MOD am 08:30   **MassIVE.quant: a community resource of curated quantitative mass spectrometry-based proteomics datasets**; Meena Choi[1]; Jeremy Carver[2]; Cristina Chiva[3, 4]; Manuel Tzouros[5]; Ting Huang[1]; Tsung-Heng Tsai[1]; Benjamin Pullman[6]; Oliver M. Bernhardt[7]; Ruth Hüttenhain[8]; Guo Ci Teo[9]; Maria Pavlou[10]; Erik Verschueren[8]; Bernd Wollscheid[10]; Alexey I. Nesvizhskii[9]; Lukas Reiter[7]; Tom Dunkley[5]; Eduard Sabido[3, 4]; Nuno Bandeira[6]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]University of California San Diego, San Diego, La Jolla, CA; [3]Barcelona Institute of Science and Technology, Barcelona, Spain; [4]Proteomics Unit, Center for Genomic Regulation, Universitat Pompeu Fabra, Barcelona, Spain; [5]Roche Pharma Research and Early Development, Pharmaceutical Sciences, Roche Innovation Center Basel, Basel, Switzerland; [6]University of California San Diego, San Diego, CA; [7]Biognosys, Schlieren, Switzerland; [8]University of California San Francisco, San Francisco, CA; [9]University of Michiagan, Ann Arbor, MI; [10]Institute of Molecular Systems Biology, Zürich, Switzerland*

MOD am 08:50   **Millisecond informatics: real-time analytics for quantitative proteomics**; Devin K Schweppe[1, 2]; Edward L Huttlin[1]; Ramin Rad[1]; Qing Yu[1]; Jimmy K Eng[2]; Jose Navarrete-Perea[1]; Joao A Paulo[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]University of Washington, Seattle, WA*

MOD am 09:10   **A Novel Method for Detection of Differential Alternative Splicing in MS Proteomics Data**; Constantin Ammar[1]; Gergely Csaba[1]; Markus Gruber[1]; Ralf Zimmer[1]; *[1]Ludwig-Maximilians-Universität München, Munich, Germany*

MOD am 09:30   **Deep neural network embedding for efficient repository-scale analysis of hundreds of millions of mass spectra**; Wout Bittremieux[1]; Damon May[2]; Jeffery A. Bilmes[2]; William Stafford Noble[2]; *[1]UCSD, La Jolla, CA; [2]University of Washington, Seattle, WA*

MOD am 09:50   **Peptide grouping within protein coding genes: A proteoform tolerant model for protein quantification in bottom-up proteomics**; Deanna L Plubell[1]; Kianna Hales[1]; Jea Park[1]; Lukas Kall[2]; Gennifer Merrihew[1]; Thomas J. Montine[3]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Royal Institute of Technology, Stockholm, Sweden; [3]Stanford University, Palo Alto, CA*

MOD am 10:10   **Extending Prosit to the prediction of proteotypicity, precursor ion charge and ion mobility collisional cross sections**; Tobias Schmidt[1]; Michael Graber[1]; Siegfried Gessulat[1]; Daniel P Zolg[1]; Tobias Rohde[2]; Brendan Maclean[2]; Patroklos Samaras[1]; Johannes Zerweck[3]; Tobias Knaute[3]; Bernard Delanghe[4]; Andreas Huhmer[5]; Karsten Schnatbaum[3]; Ulf Reimer[3]; Bernhard Kuster[1]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]University of Washington, Seattle, WA; [3]JPT Peptide Technologies GmbH, Berlin, Germany; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA*

MOE am: Microorganisms and the Microbiome

Chair: Vanessa Phelan (University of Colorado, Denver - Anschutz)

MOE am 08:30 **Combatting fungal infections through the discovery and elucidation of novel anti-virulence strategies**; Brianna Ball[1]; Duncan Carruthers-Lay[1]; Elizabeth Woroszchuk[1]; Jennifer Geddes-McAlister[1]; [1]*University of Guelph, GUELPH, ON*

MOE am 08:50 **Proteomics Reveal the Underlying Mechanisms of Filamentous Persisters during Ampicillin Treatment and Resuscitation**; Jordy Evan Sulaiman[1]; Henry Lam[1]; [1]*The Hong Kong University of Science and Technology (HKUST), Clear Water Bay, Hong Kong*

MOE am 09:10 **Minimum Inhibitory Concentration Determined by Incorporation of Deuterium in Microbial Lipids**; Matthew Sorensen[1]; Francesca Gardener[2]; David R Goodlett[3, 4]; Robert K Ernst[2]; Erik Nilsson[1]; [1]*Pataigin, LLC, Baltimore, MD; [2]University of Maryland, Baltimore, Baltimore, MD; [3]University of Maryland, Baltimore, MD; [4]International Centre for Cancer Vaccine Science, Gdansk, Poland*

MOE am 09:30 **Deciphering Host Immune Responses to Staphylococcus aureus Infection by Combining Imaging Mass Spectrometry and CODEX Multiplexed Immunofluorescence**; Elizabeth Kathleen Neumann[1, 2]; Nathan Heath Patterson[1, 3]; Jamie L Allen[2]; Jessica R Sheldon[4]; David M Anderson[1, 2]; Richard M. Caprioli[1, 2, 5]; Eric P Skaar[4, 6]; Jeffrey M. Spraggins[1, 2, 7]; [1]*Department of Biochemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University, Nashville`, TN; [5]Department of Chemistry, nashville, TN; [6]Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN*

MOE am 09:50 **Unravelling chemical mechanisms in microbial interactions by combining thin layer chromatography, ion mobility and MALDI imaging mass spectrometry**; Andréa Mccann[1]; Christopher Kune[1]; Raphaël La Rocca[1]; Janina Oetjen[2]; Anthont Arguelles Arias[3]; Marc Ongena[3]; Johann Far[1]; Gauthier Eppe[1]; Loic Quinton[4]; Edwin De Pauw[1]; [1]*University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium; [4]University of Liege, Liège, Belgium*

MOE am 10:10 **A Galaxy-based meta-omic approach for characterizing microbiome functional dynamics via integrated metaproteomics and metatranscriptomics abundance analysis**; Pratik Dilip Jagtap[1]; Praveen Kumar[1]; Marie A Crane[2]; Subina Mehta[1]; James E Johnson[1]; Thomas Mcgowan[1]; Magnus O Arntzen[3]; Francesco Delogu[3]; Ray Sajulga[1]; Srikant Verma[4]; Krishanpal Anamika[4]; Timothy J Griffin[1]; [1]*University of Minnesota, Minneapolis, MN; [2]Macalester College: Private Liberal Arts College, St. Paul, Minnesota; [3]Norwegian University of Environmental and Life Sciences, Ås, Norway; [4]Persistent Systems Limited, Pune, India*

MOF am: Biomarkers: Quantitative Analysis

Chair: Brian Rago (Pfizer)

MOF am 08:30 **Development and qualification of a novel offline SPE and MRM method to quantify eicosanoids and related PUFAs**; Monika Mital Kansal[1]; Veronica Anania[1]; Rod Mathews[1]; Olga Li[1]; [1]*Genentech, South San Francisco, CA*

MOF am 08:50 **Improving the Diagnosis and Treatment CKD-MBD using a UHPLC-HRMS Reference Measurement Procedure for Parathyroid Hormone**; Candice Z. Ulmer[1]; Sarah Kingsley[2]; Bianca Smith[2]; Janet Thonkulpitak[3]; Hubert W. Vesper[4]; [1]*Centers for Disease Control and Prevention, Atlanta, GA; [2]Battelle, Columbus, Ohio; [3]Oak Ridge Institute for Science and Education (ORISE) Participant Program, Oak Ridge, Tennessee; [4]Centers For Disease Control and Prevention, Atlanta, GA*

MOF am 09:10 **Quantitative MHC-I peptide measurement to support the development of cancer immunotherapeutic approaches using Parallel Reaction Monitoring**; Vittoria Massafra[1]; Sabine Kux Van Geijtenbeek[2]; Martin Steegmaier[3]; Yvonne Alice Nagel[4]; Axel Ducret[2]; [1]*Roche Pharma Research and Early Development, Discovery Oncology, Roche Innovation Center Basel, Basel, Switzerland; [2]Roche Pharma Research and Early Development, Pharmaceutical Sciences, Roche Innovation Center Basel, Basel, Switzerland; [3]Roche Pharma Research and Early Development, Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany; [4]Roche Pharma Research and Early Development, Discovery Oncology, Roche Innovation Center, Basel, Switzerland*

MOF am 09:30 **A High Throughput Antibody-free Platform for Multiplexed, Sensitive Quantification of Protein Biomarkers in Complex Biomatrices**; Bo An[1]; Timothy Sikorski[1]; Tujin Shi[2]; Yuqian Gao[2]; Jon Jacobs[2]; Matthew Szapacs[1]; [1]*GSK, Collegeville, PA; [2]PNNL, Richland, WA*

MOF am 09:50 **A GCLP Quantitative Mass Spectrometry Workflow for Multiplexed Measurement of Protein Biomarkers in FFPE Tissues**; Michael Schirm; *Caprion Biosciences Inc., Montreal, QC*

MOF am 10:10   **Applying high-throughput proteomics technology to discover biomarkers of liver disease**; Lili Niu[1, 2]; Florian Meier[2]; Philipp Geyer[1, 2]; Nicolai Jacob Wewer Albrechtsen[1, 3]; Alberto Santos Delgado[1]; Rajat Gupta[1]; Maja Thiele[4, 5]; Aleksander Krag[4, 5]; Jonel Trebicka[6]; Matthias Mann[1, 2]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; [2]Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Department of Clinical Biochemistry, Rigshospitalet, University of Copenhagen, Copenhagen N, Denmark; [4]Department of Gastroenterology and Hepatology and OPEN, Odense Patient data Explorative Network, Odense University Hospital, Odense C, Denmark; [5]Institute of Clinical Research, University of Southern Denmark, Odense C, Denmark; [6]Department of Medicine I, University of Frankfurt, Frankfurt, Germany*

MOG am: Environmental: Innovative Approaches and Instrumentation

Chair: Achille Cappiello (University of Urbino)

MOG am 08:30   **Quantitative non-targeted LC/HRMS analysis for water and food monitoring**; Anneli Kruve[1]; Jaanus Liigand[2]; Andrea Mizzi Brunner[3]; Tingting Wang[4]; Jon R Sobus[5]; Louis C Groff[5]; Karin Kiefer[6]; Juliane Hollender[6]; *[1]Stockholm University, Stockholm, Sweden; [2]University of Tartu, Institute of Chemistry, Tartu, Estonia; [3]KWR Water Research Institute, Utrecht, Netherlands; [4]Technical University of Denmark, Lyngby, Denmark; [5]United States Environmental Protection Agency, Durham, NC; [6]EAWAG, Duebendorf, Switzerland*

MOG am 08:50   **Concurrent Electron and Proton Chemical Ionization of Polyaromatic Hydrocarbons via the Liquid Sampling–Atmospheric Pressure Glow Discharge (LS-APGD) Ionization Source**; R. Kenneth Marcus[1]; Jacob R. Bills[1]; Tyler J. Williams[1]; *[1]Clemson University, Clemson, SC*

MOG am 09:10   **Micropollutants distribution using MALDI Imaging in a whole reed plant growing in a polluted environment**; Loïc Maurer[1, 2]; Claire Villette[2]; Adrien Wanko[1]; Dimitri Heintz[2]; *[1]Département mécanique des fluides et rhéologie, ICube Laboratoire des sciences de l'ingénieur, de l'informatique et de l'imagerie, UNISTRA/CNRS/ENGEES/INSA, Strasbourg, France; [2]Plant Imaging and Mass Spectrometry (PIMS), Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, STRASBOURG, France*

MOG am 09:30   **Molecular Reconstruction and Analysis of Organic-Aerosol Composition from a High-alpine Glacier Ice Core Covering the Pre-industrial to the Present-day Transition**; Alexander Vogel[1, 2]; Franziska Bachmeier[2]; Anja Lauer[2]; Katarzyna Arturi[2]; Urs Baltensperger[3]; Imad El Haddad[3]; Margit Schwikowski-Gigar[3]; Sasa Bjelic[1]; *[1]Paul Scherrer Institute (PSI), Villigen PSI, Switzerland; [2]Goethe-Universität, Frankfurt am Main, Germany; [3]Paul Scherrer Institute (PSI), Villigen, Switzerland*

MOG am 09:50   **On-Site Perfluorocarbon Tracer Detection with a Coded Aperture Miniature Mass Spectrometer**; Kathleen L Horvath[1]; Tanouir Aloui[2]; Raul Vyas[2]; Elettra Piacentino[2]; Rafael Bento Serpa[2]; Maria Luisa Sartorelli[2]; Jason J Amsden[2]; Jeffrey T. Glass[2]; Roger P Sperline[3]; M. Bonner Denton[3]; Jesko Von Windheim[2]; David Koester[2]; Patrick Keelan[4]; Yuriy Zhilichev[5]; *[1]Duke University, Durham, NC; [2]Duke University, Durham; [3]University of Arizona, Tucson, AZ 85351; [4]PFT Technology LLC., Belleview, NY; [5]Consultant, Durham, North Carolina*

MOG am 10:10   **Empty Slot.** Stay tuned for promoted selection to be made.

MOH am: Fundamentals: Ion Spectroscopy

Chair: Jean-Yves Salpin (CNRS - University of Evry)

MOH am 08:30   **Novel LC - Infrared Ion Spectroscopy Approaches for the Structure Elucidation of Biomarkers**; Fred A. M. G. Van Geenen[1, 2]; Udo F. Engelke[2]; Rianne E. Van Outersterp[1]; Kas J. Houthuijs[1]; Giel Berden[1]; Ron A. Wevers[2]; Karlien L. M. Coene[2]; Jonathan Martens[1]; Jos Oomens[1, 3]; *[1]Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Nijmegen, Netherlands; [2]Department of Laboratory Medicine, Translational Metabolic Laboratory, Radboud University Medical Center, Nijmegen, Netherlands; [3]van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Netherlands*

MOH am 08:50   **Intrinsic Effects of Fluorine Substitutions on the Structures and Glycosidic Bond Stabilities of Protonated Cytidine Analogues**; Mary T Rodgers[1]; Zachary J. Devereaux[1]; Harrison A. Roy[1]; Lucas A. Hamlow[1]; Chenchen He[1]; Yanlong Zhu[1]; Erik O. Soley[1]; Nathan A. Cunningham[1]; Giel Berden[2]; Jos Oomens[2]; *[1]Wayne State University, Detroit, MI; [2]Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Nijmegen, Netherlands*

MOH am 09:10   **Leveraging High-Resolution Mass Spectrometry and Cryogenic Vibrational Infrared Spectroscopy to Capture Intermediates in Small Molecule Activation: Applications to Nickel(I)**; Evan H Perez[1]; Sean C Edington[1]; Fabian S Menges[1]; Mark A Johnson[1]; *[1]Yale University, New Haven, CT*

MOH am 09:30   **Reforming the Single-TurnAlpha Helix: Cold Ion Spectroscopy of Novel Cyclic Peptide Ions**; John Lawler[1]; Timothy Hill[2]; David Fairlie[2]; Timothy Zwier[3]; Scott A. Mcluckey[1]; *[1]Purdue University, West Lafayette, IN; [2]University of Queensland, St Lucia, Australia; [3]Sandia National Laboratories, Livermore, California*

MOH am 09:50   **UV/Vis Photodissociation Action Spectroscopy of Ionized DNA Components. Adenine and 9-Methyladenine Cation Radicals in the Gas-Phase**; Shu R. Huang[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

MOH am 10:10   **Combined FAIMS, picosecond laser PD and ion trap MS reveals differences in the photostability of selected deprotonation isomers of FAD2-**; Samuel Marlton[1]; Ben I. Mckinnon[1]; Boris Ucur[1]; Stephen J. Blanksby[2]; Adam J. Trevitt[1]; *[1]University of Wollongong, Wollongong, Australia; [2]Queensland University of Technology, Brisbane, Australia*

MOA pm: Clinical Analysis : Applications
Chair: Therese Koal (Biocrates)

MOA pm 02:30   **Application of a Molecular Networking Approach combined with MetWork web server for Therapeutic Drug Monitoring and Toxicology**; Emmanuel Bourgogne[1, 2]; Christel Grondin[3]; Sophie Magréault[4]; Yann Beauxis[5]; Grégory Genta-Jouve[5, 6]; *[1]Université de Paris, Faculté de Pharmacie, Paris, France; [2]APHP, Hopital Saint Antoine, UF Suivi THérapeutique du Médicament, Paris, France; [3]APHP, Hopital Lariboisiere, UF Toxicologie, Paris, France; [4]APHP, Hopital Jean Verdier, UF Pharmacologie, Bondy, France; [5]CNRS UMR8038, Paris, France; [6]USR 3456 CNRS LEEISA, Cayenne, France*

MOA pm 02:50   **Tissue Identification and Diagnosis in Human Surgeries using the MasSpec Pen Technology**; Jialing Zhang[1]; Marta Sans[1]; Rachel J. DeHoog[1]; Kyana Garza[1]; Mary King[1]; Clara L Feider[1]; Alena Bensussan[1]; Michael F. Keating[1]; Anna C. Krieger[1]; Sunil P Badal[1]; John Lin[1]; Wendong Yu[2]; Chandandeep Nagi[2]; Chris Pirko[1]; Kirtan Brahmbhatt[2]; Thomas E. Milner[1]; Sadhna Dhingra[2]; George Van Buren[2]; Stacey A Carter[2]; William E Fisher[2]; Omar Barakat[2]; Raymon Grogan[2]; James Suliburk[2]; Livia S. Eberlin[1]; *[1]UT Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX*

MOA pm 03:10   **Identification and characterization of antithrombin deficiency in patients using a targeted mass spectrometry based clinical chemistry test**; Renee Ruhaak[1]; María Eugenia De La Morena-Barrio[2]; Fred P.H.T.M. Romijn[1]; Mervin M. Pieterse[1]; Maarten P.J. Van Hoorn[1]; Javier Corral[2]; Christa M. Cobbaert[1]; *[1]Department of Clinical Chemistry and Laboratory Medicine, Leiden University Medical Center, Leiden, Netherlands; [2]Servicio de Hematología y Oncología Médica, Hospital Universitario Morales Meseguer, Centro Regional de Hemodonación, Universidad de Murcia, IMIB-Arrixaca, Murcia, Spain*

MOA pm 03:30   **Multi-Center Assessment of Tumor Classification Reproducibility by MALDI Imaging**; Soeren-Oliver Deininger[1]; Tobias Boskamp[1]; Christine Bollwein[2]; Rita Casadonte[3]; Petra Wandernoth[3]; Katharina Kriegsmann[4]; Mark Kriegsmann[5]; Jörg Kriegsmann[3]; Wilko Weichert[2]; Peter Schirmacher[5]; Alice Ly[1]; Kristina Schwamborn[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Institute of Pathology, Technical University Munich, Munich, Germany; [3]Proteopath GmbH, Trier, Germany; [4]Department of Hematology, Oncology and Rheumatology, University Hospital Heidelberg, Heidelberg, Germany; [5]Institute of Pathology, University Hospital Heidelberg, Heidelberg, Germany*

MOA pm 03:50   **Fatty liver is more than "fat accumulation": shotgun lipidomics of human non-alcoholic fatty liver disease and steatohepatitis**; Olga Vvedenskaya[1]; Oskar Knittelfelder[1]; Alessandra Palladini[2]; Judith Wodke[3]; Tim Rose[4]; Eduardo Jacobo Miranda Ackerman[1]; Veera Raghavan Thangapandi[5]; Mario Brosch[5]; Edda Klipp[3]; Josch Pauling[4]; Jochen Hampe[5, 6]; Andrej Shevchenko[1]; *[1]Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany; [2]Paul Langerhans Institute Dresden of the Helmholtz Zentrum Munich at the University Clinic Carl Gustav Carus, Dresden, Germany; [3]Humboldt University, Berlin, Germany; [4]Technische Universität München, LipiTUM, Munich, Germany; [5]Medizinischen Klinik 1 Bereich Gastroenterologie & Hepatologie, Universitätsklinikum, Dresden, Germany; [6]Center for Regenerative Therapies, Dresden, Germany*

MOA pm 04:10   **Dilution in Situ for LC-MS/MS Workflows in Diagnostic Assays**; Christine Gomes[1]; Matthew T Campbell[1]; Brian Rappold[1]; *[1]LabCorp, Raleigh, NC*

MOB pm: Exposomics, Toxicology, and Health Outcomes
Chair: Benedikt Warth (University of Vienna)

MOB pm 02:30   **Analyzing the Exposome: Perioperative environmental exposure to cyclohexanone during neonatal congenital cardiac surgery is associated with decreased neurodevelopmental outcomes**; Allen Everett[1]; Jessie Buckley[2]; Greg Ellis[3]; Jun Yang[4]; David R Graham[2]; Eric Graham[5]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD; [2]Johns Hopkins University, Baltimore, MD; [3]Johns Hopkins All Children's Hospital, St. Petersburg, 33701; [4]Johns Hopkins School of Medicine, Baltimore, MD; [5]Medical University of South Carolina, Department of Biochemistry and Molecular Biology, Charleston, SC*

MOB pm 02:50   **Metabolomics and Proteomics Analysis of the Effects of Vinclozolin Exposure in Utero on Dams and Fetuses**; Alana Rister[1]; Ciro M. Amato[1, 2]; Joshua P. Mogus[1]; Kimberly A. Kew[1]; Krista A. Mccoy[1]; *[1]East Carolina University, Greenville, North Carolina; [2]National Institute of Environmental Health Sciences, Durham, North Carolina*

MOB pm 03:10   **Reactomics: using mass spectrometry as a reaction detector**; Miao Yu[1]; Lauren Petrick[1]; *[1]Icahn School of Medicine at Mount Sinai, New York, NY*

MOB pm 03:30   **Targeted and Untargeted Screening of DNA Adducts in the Genome of Prostate Cancer Patients**; Jingshu Guo[1]; Scott J Walmsley[1]; Haoqing Chen[1]; Peter W. Villalta[1]; Paari Murugan[1]; Christopher J Weight[1]; Robert J Turesky[1]; *[1]University of Minnesota, Minneapolis, MN*

MOB pm 03:50   **Pan-albumin adductomics: Untargeted detection of electrophilic adducts at multiple residues of serum albumin for discovery and characterization of environmental exposures**; Joshua W Smith[1]; Robert N

O'Meally[1]; Conor Jenkins[2]; Derek Ng[1]; Thomas W Kensler[1, 3]; Robert N Cole[1]; John D Groopman[1]; [1]*Johns Hopkins University, Baltimore, MD;* [2]*US Army Public Health Center, Aberdeen Proving Ground, MD;* [3]*Fred Hutchinson Cancer Research Center, Seattle, WA*

MOB pm 04:10   **Empty Slot.** Stay tuned for promoted selection to be made.

MOC pm: Drug Discovery and Development: Quantitative Analysis
Chair: Michael G. Bartlett (University of Georgia)

MOC pm 02:30   **iBA – intelligent Bioanalysis, Striving Towards the Lab of the Future**; Frank Runge[1]; Svenja Mayer-Wrangowski[1]; Tom Bretschneider[1]; Siegfried Wild[1]; Anne-Michaela Kübler[1]; Wolfgang Jörg[2]; Jürgen Weber[2]; Christian Späth[2]; Andreas H Luippold[1]; [1]*Boehringer Ingelheim, Drug Discovery Sciences, Biberach an der Riss, Germany;* [2]*Boehringer Ingelheim, Site Engineering and Technology, Biberach an der Riss, Germany*

MOC pm 02:50   **Multiplexed Chemical Proteomics for Cell-based Screening of Large Electrophile Libraries**; Miljan Kuljanin[1]; Dylan C Mitchell[1]; Devin K Schweppe[1]; Ajami S Gikandi[2]; David P Nusinow[1]; Joseph D Mancias[2]; Steven P Gygi[1]; [1]*Harvard Medical School, boston, MA;* [2]*Dana-Farber Cancer Institute/ Harvard Medical School, Boston, MA*

MOC pm 03:10   **HCP Analysis by Internal Standard-Triggered Assay of a Panel of Heavy Tryptic Peptides of the Most Common and Troublesome CHO-HCPs**; Andrew D Mahan[1]; Eric Beil[2]; Hirsh Nanda[2]; Bhavin Patel[3]; Sebastien Gallien[4, 5]; Aaron S. Gajadhar[6]; [1]*Johnson and Johnson, Spring House, PA;* [2]*Janssen Pharmaceuticals R&D, Spring House, PA;* [3]*Thermo Fisher Scientific, Rockford, IL;* [4]*Thermo Fisher Scientific, Paris, France;* [5]*Thermo Fisher Scientific, Cambridge Proteomics Research Group, Cambridge, MA;* [6]*Thermo Fisher Scientific, San Jose, CA*

MOC pm 03:30   **Profiling of Human iPSC-Derived NGN2 Neurons During Differentiation by Quantitative Proteomics**; Dirk Walther[1]; Naomi Okugawa[1]; Sandi Engle[1]; Ru Wei[1]; [1]*Biogen, Cambridge, MA*

MOC pm 03:50   **Empty Slot.** Stay tuned for promoted selection to be made.

MOC pm 04:10   **Empty Slot.** Stay tuned for promoted selection to be made.

MOD pm: Informatics: Metabolomics
Chair: Kendra Adams (Duke University)

MOD pm 02:30   **CFM-ID 4.0: Substantially improved fragmentation algorithm and extended rules-based coverage of predicting ESI MS/MS spectra**; Fei Wang[1]; Jaanus Liigand[2, 3]; David Arndt[2]; Russ Greiner[4]; David S Wishart[1, 2]; [1]*Department of Computing Science, University of Alberta, Edmonton, AB;* [2]*Department of Biological Sciences, University of Alberta, Edmonton, AB;* [3]*University of Tartu, Institute of Chemistry, Tartu, Estonia;* [4]*Department of Computing Science, University of Alberta, Edmonton, AB T6G 2E8, Canada, Edmonton, AB*

MOD pm 02:50   **Developing a Data Processing Pipeline for Extending a Comprehensive Tandem Mass Spectral Library**; Xiaoyu Yang[1]; Pedatsur Neta[1]; Yuxue Liang[1]; Connie A. Remoroza[1]; Yamil Simón-Manso[1]; Kelly H. Telu[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Alexey Mayorov[1]; Tytus D. Mak[1]; Lewis Y. Geer[1]; Stephen E. Stein[1]; [1]*National Institute of Standards and Technology, Gaithersburg, Maryland*

MOD pm 03:10   **Machine learning methods for METASPACE, an AI platform for spatial metabolomics**; Theodore Alexandrov[1, 2]; Katja Ovchinnikova[1]; Lachlan Stuart[1]; Christopher M. Baxter Rath[1, 3]; Vitaly Kovalev[1]; Veronika Saharuka[1]; Alexander Rakhlin[4]; Sergey Nikolenko[4, 5]; [1]*EMBL – European Molecular Biology Laboratory, Heidelberg, Germany;* [2]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA;* [3]*Ometa Labs, San Diego, CA;* [4]*Neuromation OU, Tallinn, Estonia;* [5]*Steklov Institute of Mathematics, St.Petersburg, Russia*

MOD pm 03:30   **Combining biological and chemical information in compound annotation for untargeted metabolomics**; Oliver Fiehn[1]; Clayton Bloszies[1]; Dinesh K. Barupal[1]; Jacob Folz[1]; Ivana Blazenovic[1]; Tobias Kind[1]; Tomas Cajka[1]; Paolo Bonini[2]; Hiroshi Tsugawa[3]; [1]*UC Davis, Davis, CA;* [2]*NGAlab, Tarragona, Spain;* [3]*RIKEN Center for Sustainable Resource Science, Yokohama, Japan*

MOD pm 03:50   **Beyond the Top Hit: Extracting Unknown Structural Information from Hybrid Similarity Search Hit Lists**; Brian T. Cooper[1, 2]; Tytus D. Mak[2]; Stephen E. Stein[2]; [1]*UNC Charlotte, Charlotte, NC;* [2]*NIST, Gaithersburg, MD*

MOD pm 04:10   **Empty Slot.** Stay tuned for promoted selection to be made.

	MOE pm: MS of Really Big Ions
	Chair: Kathrin Breuker (University of Innsbruck)

MOE pm 02:30   **Megadalton Mosaics: Assembling Molecular Information Piece by Piece using Charge Detection Mass Spectrometry**; <u>Conner C Harper</u>[1]; Evan R Williams[1]; [1]*University of California, Berkeley, Berkeley, CA*

MOE pm 02:50   **Assessing DNA packaging in individual virophage virions using charge independent nano-mechanical MS**; <u>Christophe Masselon</u>[1]; Szu-Hsueh Lai[1]; Sandra Jeudy[2]; Bogdan Vysotskyi[1]; Kavya Clement[1]; Lionel Bertaux[2]; Marc Gely[3]; Lucid Belmudes[1]; Jean-Michel Claverie[2]; Yohann Coute[1]; Sébastien Hentz[3]; Chantal Abergel[2]; [1]*CEA, IRIG, Biologie à Grande Echelle, Grenoble, France; [2]Aix-Marseille University, CNRS UMR 7283, Marseille, France; [3]Université Grenoble Alpes, CEA, LETI, Grenoble, France*

MOE pm 03:10   **Charge Detection Mass Spectrometry Measurements of Exosomes and other Extracellular Particles Enriched from Bovine Milk**; <u>Brooke A Brown</u>[1]; Xuyao Zeng[1]; Aaron Todd[1]; Lauren Frances Barnes[1]; Jonathan Winstone[1]; Jonathan C. Trinidad[1]; Milos V. Novotny[1]; Martin F. Jarrold[1]; David E. Clemmer[1]; [1]*Indiana University, Bloomington, IN*

MOE pm 03:30   **Mass and charge distributions of entire amyloid fibers by charge detection mass spectrometry: mapping heterogeneity and polymorphism**; <u>Mohammad Abdul Halim</u>[1]; Jonathan Pansieri[2]; Philippe Dugourd[3]; Vincent Forge[4]; Rodolphe Antoine[3]; [1]*University of Arkansas Fort Smith, Fort Smith, AR; [2]Nuffield Department of Clinical Neurosciences, Oxford University, Oxford, United Kingdom; [3]Institut Lumière Matière CNRS et Université Lyon 1, LYON, France; [4]Laboratoire Chimie et Biologie des Métaux CEA-Grenoble, Grenoble, France*

MOE pm 03:50   **Resolving heterogeneous macromolecular assemblies by Orbitrap-based (UHMR) single particle charge-detection mass spectrometry (CD-MS)**; <u>Tobias P. Wörner</u>[1, 2]; Joost Snijder[1, 2]; Antonette Bennett[3]; Mavis Agbandje-McKenna[3]; Thomas W. Powers[4]; Olga V. Friese[4]; Alexander A. Makarov[1, 5]; Albert J.R. Heck[1, 2]; [1]*Biomolecular Mass Spectrometry and Proteomics, Faculty of Science, Utrecht University, 3584 CH Utrecht, Netherlands; [2]Netherlands Proteomics Center, Padualaan 8, Netherlands; [3]Department of Biochemistry and Molecular Biology, Center for Structural Biology, the McKnight Brain Institute, 1200 Newell Drive, Gainesville, FL 32610; [4]BioTherapeutics Pharmaceutical Sciences, Pfizer, Inc, Chesterfield, MO 63017; [5]Thermo Fisher Scientific, Bremen, Germany*

MOE pm 04:10   **From Human Nucleosomes to Virus-Like Particles:Multiplexing the Orbitrap to Readout Individual Ion Mass Spectra**; <u>Jared Kafader</u>[1]; Rafael D Melani[1]; Luis Schachner[1]; Kenneth R Durbin[1]; Bon Ikwuagwu[1]; Bryan P Early[1]; Ryan T Fellers[1]; Steven C Beu[2]; Vlad Zabrouskov[3]; Joshua T Maze[4]; Deven L Shinholt[4]; Ping F. Yip[3]; Danielle Tullman-Ercek[1]; Michael W. Senko[3]; Philip D. Compton[1]; Neil L. Kelleher[1]; [1]*Northwestern University, Evanston, IL; [2]S.C. Beu Consulting, Austin, Texas; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Austin, TX*

	MOF pm: Post-translational Modifications: Qualitative & Quantitative Analysis
	Chair: Luca Fornelli (University of Oklahoma)

MOF pm 02:30   **Mapping ADP-ribosylation using Activated Ion Electron Transfer Dissociation (AI-ETD)**; <u>Sara C Buch-Larsen</u>[1, 2]; Ivo A Hendriks[1, 2]; Jean M Lodge[3]; Martin Rykær[1]; Benjamin Furtwängler[1]; Evgenia Shishkova[3]; Michael S. Westphall[3]; Joshua J Coon[3]; Michael L Nielsen[1]; [1]*Novo Nordisk Foundation Center for Protein Research, København, Denmark; [2]Equal contribution, ., Denmark; [3]University of Wisconsin-Madison, Madison, Wisconsin*

MOF pm 02:50   **Identification and characterization of a new protein post-translational modification, lysine lactylation, by mass spectrometry-based proteomics approaches**; Di Zhang[1]; Zhanyun Tang[2]; He Huang[1]; Guolin Zhou[1]; Mathew Perez-Neut[1]; Robert G. Geoder[2]; Lev Becker[1]; <u>Yingming Zhao</u>[1]; [1]*Ben May Department for Cancer Research, The University of Chicago, Chicago, Illinois; [2]Laboratory of Biochemistry and Molecular Biology, The Rockefeller University, New York, NY*

MOF pm 03:10   **From single cell to single embryo: Unraveling protein phosphorylation dynamics of the early cell cycle**; <u>Juan M Valverde</u>[1, 2]; Liliana Krasinska[3]; Daniel Fisher[3]; Albert J.R. Heck[1, 2]; Puck Knipscheer[4]; Maarten Altelaar[1, 2]; [1]*Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands; [3]Montpellier Institute of Molecular Genetics, Montpellier, France; [4]Oncode Institute, Hubrecht Institute–KNAW and University Medical Center, Utrecht, Netherlands*

MOF pm 03:30   **Quantification of thermal stability of intact proteoforms using quantitative top-down proteomics**; <u>Kellye A Cupp-Sutton</u>[1]; Thomas Welborn[1]; Si Wu[1]; [1]*University of Oklahoma, Norman, OK*

MOF pm 03:50   **Quantitative Top-Down Proteomics reveals the Distinct Substrate Specificity of p300 and CBP**; <u>Tao Wang</u>[1]; Matthew V. Holt[1]; Nikit Venishetty[2]; Nicolas L. Young[3]; [1]*Baylor College of Medicine, Houston, TX; [2]Rice University, Houston, TX; [3]Baylor College of Medicine, Houston*

MOF pm 04:10   **Empty Slot.** Stay tuned for promoted selection to be made.

MOG pm 02:30 **Single injection LC-HRMS large-scale quantitative metabolomics using multipoint internal calibration and on-demand produced multideuterated metabolites**; Kathleen Rousseau[1]; Jessica Michieletto[1]; Yu Min Kiw[1]; Sophie Feuillastre[2]; Grégory Pieters[2]; Christophe Junot[1]; François Fenaille[1]; Annelaure Damont[1]; [1]*Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France;* [2]*Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), Gif-sur-Yvette, France*

MOG pm 02:50 **Detection of Lipogenesis at Very High Sensitivity Using Orbitrap Gas Chromatography High-resolution Mass Spectrometry**; Xiaorong Fu[1]; Stanisław Deja[1]; Justin Fletcher[1]; Norma Anderson[1]; Matthew Mitsche[1]; Goncalo Vale[1]; Jeffrey Mcdonald[1]; Jay Horton[1]; Shawn Burgess[1]; [1]*UT Southwestern Medical Center, Dallas, TX*

MOG pm 03:10 **Use of stable isotope-labeled peptidic drugs to facilitate metabolite identification for sports drug testing purposes**; Mario Thevis[1]; Andreas Thomas[1]; [1]*German Sport University, Cologne, Germany*

MOG pm 03:30 **Methylation dynamics of histone H3.3K27me3 in pluripotency and differentiation of embryonic stem cells**; Yekaterina Kori[1]; Simone Sidoli[1, 2]; Zuo-Fei Yuan[1, 3]; Benjamin A. Garcia[1]; [1]*University of Pennsylvania, Philadelphia, PA;* [2]*Albert Einstein College of Medicine, The Bronx, NY;* [3]*St. Jude Children's research hospital, Memphis, TN*

MOG pm 03:50 **In vivo Protein Turnover Rates Across the Proteome for Various Mouse Tissues**; Zach Rolfs[1]; Brian L Frey[1]; Xudong Shi[2]; Yoshitaka Kawai[2]; Lloyd M Smith[1]; Nathan V Welham[2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Surgery, University of Wisconsin-Madison, Madison, WI*

MOG pm 04:10 **Analysis of Isotopically-Depleted Proteins Derived from Bacterial Cells by 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Zeljka Popovic[1]; Lissa C. Anderson[2]; Xuepei Zhang[3]; David S. Butcher[2]; Greg T. Blakney[2]; Roman Zubarev[3]; Christopher L. Hendrickson[1, 2]; Alan G. Marshall[1, 2]; [1]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL;* [2]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [3]*Karolinska Institute, Solna, Sweden*

MOH pm 02:30 **Desalting proteins using infrared photoactivation**; Jean M Lodge[1]; Michael S Westphall[1]; Joshua J Coon[1]; [1]*University of Wisconsin, Madison, WI*

MOH pm 02:50 **Gas-phase separation and concentration of phosphatidylcholine lipids using charge inversion ion/ion reactions enabled on an FT-ICR mass spectrometer**; Jonathan T Specker[1]; Boone M. Prentice[1]; [1]*University of Florida, Gainesville, FL*

MOH pm 03:10 **CID Tandem MS and Traveling Wave IMS to Investigate Non-Covalent Interactions for Asymmetric Catalysis**; Dr. Ulrike Warzok[1]; Banruo Huang[1]; Dr. Anthony T. Iavarone[1]; Prof. F. Dean Toste[1]; [1]*University of California, Berkeley, Berkeley, CA*

MOH pm 03:30 **Simple and minimally invasive SID devices for native mass spectrometry**; Dalton Snyder[1]; Erin Panczyk[1]; Ben Jones[1]; Arpad Somogyi[1]; Desmond Kaplan[2]; Vicki Wysocki[1]; [1]*The Ohio State University, Columbus, OH;* [2]*KapScience LLC, TEWKSBURY, MA*

MOH pm 03:50 **Selective gas-phase ion/ion chemistries for the structural elucidation of complex lipids in direct infusion workflows**; Caitlin E. Randolph[1]; De'shovon M. Shenault[1]; Kimberly C. Fabijanczuk[1]; Reuben S. E. Young[2]; Stephen J. Blanksby[2]; Scott A. Mcluckey[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Queensland University of Technology, Brisbane, Australia*

MOH pm 04:10 **UVPD-FTICR-2DMS: Expanding the toolbox for biomolecule analysis**; Alina Theisen[1]; Christopher A. Wootton[1]; Anisha Haris[1]; Tomos E. Morgan[1]; Yuko Lam[1]; Sean Ellacott[1]; Sebastien Perrier[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom*

TOA am: Instrumentation: New Developments in Ionization and Sampling: In Memory of Burnaby Munson
Chair: Jeffrey McGuire (U.S. Army CCDEVCOM Chemical Biological Center)

TOA am 08:30 **A Novel NanoESI-Microreactor Ionization Source for Microwave-Assisted Bottom-Up Proteomics**; Maria E Rivera[1]; Steven J Ray[1]; [1]*University at Buffalo, Buffalo, NY*

TOA am 08:50 **On-demand ionization for miniature mass spectrometry analysis system**; Junhan Wu[1]; Wenpeng Zhang[2]; Zheng Ouyang[1]; [1]*Tsinghua University, Beijing, China;* [2]*Purdue University, West Lafayette*

TOA am 09:10 **Electron Ionization LC-MS and GC-MS Combined Instrument Using Single MS**; Svetlana Tsizin[1]; Alexander B. Fialkov[1]; Aviv Amirav[1]; [1]*Tel Aviv University, Tel Aviv, Israel*

TOA am 09:30 **Spray-capillary Based Capillary Electrophoresis Mass Spectrometry Analysis of Metabolites in Live Cells**; Lushuang Huang[1]; Zhe Wang[1]; Mulin Fang[1]; Drew King[2]; Cupp-Sutton Kellye[1]; Si Wu[1]; [1]*University of Oklahoma, Dept. of Chem & Biochem, Norman, OK;* [2]*University of Oklahoma, Norman, OK*

TOA am 09:50 **New Approaches for Efficient Sampling and Ionization in High-Resolution Imaging Using Nanospray Desorption Electrospray Ionization (nano-DESI) Mass Spectrometry**; Julia Laskin[1]; Xiangtang Li[1]; Ruichuan Yin; Daisy M Unsihuay Vila[1]; Daniela Mesa Sanchez[1]; [1]*Purdue University, West Lafayette, IN*

TOA am 10:10 **Boosting Ion Signal Levels with cVSSI for MS/MS and MSn of Biopolymers**; Kushani U Attanayake[1]; Chong Li[1]; Daud Sharif[1]; Sandra N Majuta[1]; Ahmad Kiani Karanji[1]; Anthony Debastiani[1]; Peng Li[1]; Stephen J Valentine[1]; [1]*West Virginia University, Morgantown, WV*

TOB am: Lipidomics: New MS Technologies and Applications
Chair: Komal Kedia (Merck)

TOB am 08:30 **An automated protocol for liquid-liquid extraction of blood plasma polar metabolites and lipids for mass spectrometri**; Tobias Marcus Maile[1]; Sudha Gollapudi[1]; Aleksandr Gaun[1]; Ngoc Vu[1]; José Zarvala-Solorio[1]; Ganesh Kolumam[1]; Fiona E. Mcallister[1]; Rob Keyser[1]; Bryson D. Bennett[1]; [1]*Calico LLC, South San Francisco, CA*

TOB am 08:50 **High-throughput and robust nanoflow chromatography combined with trapped ion mobility spectrometry and PASEF for in-depth lipidomics from 1µL human plasma**; Catherine G. Vasilopoulou[1]; Nicolai Bache[2]; Ole Hoerning[2]; Philipp E. Geyer[1, 3]; Karolina Sulek[3]; Andreas-David Brunner[1]; Dmitry Voytik[1]; Sanjib Meitei[4]; Aiko Barsch[5]; Matthias Mann[1, 3]; Florian Meier[1]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Evosep Biosystems, Odense, Denmark;* [3]*NNF Center for Protein Research, Copenhagen, Denmark;* [4]*PREMIER Biosoft, Indore, India;* [5]*Bruker Daltonik GmbH, Bremen, Germany*

TOB am 09:10 **A workflow to link lipid structures with biological and metadata utilizing novel visualization and clustering tools**; Melanie Odenkirk[1]; Phyo Phyo Kyaw Zin[1]; Jeremy Ash[1, 2]; David Reif[3]; Denis Fourches[1]; Erin S. Baker[1]; [1]*Department of Chemistry, North Carolina State University, Raleigh, North Carolina;* [2]*Department of Statistics, North Carolina State University, Raleigh, North Carolina;* [3]*Department of Biological Sciences, North Carolina State University, Raleigh, North Carolina*

TOB am 09:30 **Multinozzle Emitters for Shotgun Lipidomics**; Na Pi Parra[1]; Maoyin Li[1]; Pan Mao[1]; Daojing Wang[1]; [1]*Newomics Inc., Berkeley, CA*

TOB am 09:50 **Untangling and Quantifying Isomeric Molecular Gangliosides using High Throughput Structures for Lossless Ion Manipulation-MS Analyses**; Kelly Wormwood[1]; James R. Arndt[1]; Liulin Deng[1]; Anisha Yadav[1]; Stephen Krufka[1]; Daniel Debord[1]; Laura Maxon[1]; Kim Ekroos[2]; [1]*MOBILion Systems Inc., Chadds Ford, PA;* [2]*Lipidomics Consulting Ltd, Esbo, Finland*

TOB am 10:10 **ANALYSIS BY LC-MS/MS OF LIPIDS EXTRACTED USING TRIZOL REAGENT**; Rahul Deshpande[1]; Nathen Bopp[1]; William Russell[1]; [1]*Mass Spectrometry Facility, University of Texas Medical Branch (UTMB), Galveston, TX*

	TOC am: Therapeutic Proteins, Antibodies, and Antibody/Drug Conjugates
	Chair: M. Violet Lee (Genentech)

TOC am 08:30   **In vitro and in vivo biotransformation studies by intact mass analysis for novel biotherapeutics**; <u>Yunan Wang</u>[1]; Mei Han[1]; Brooke M. Rock[1]; Dan A. Rock[1]; [1]*Amgen, SSF, CA*

TOC am 08:50   **Accelerated sequence identification of functional antibodies from high throughput human B-cell screens using reversed immunocaputure / HR LC-MS2**; <u>Eberhard Durr</u>[1]; Yaping Liu[1]; Arthur Fridman[2]; Zhifeng Chen[1]; Nicole Sullivan[1]; Kristin Geddes[1]; Aimin Tang[1]; Brian Squadroni[1]; Paul Zuck[1]; [1]*Merck Research Laboratories, West Point, PA;* [2]*Merck Research Laboratories, Rahway, NJ*

TOC am 09:10   **Mapping Binding Epitopes of Bispecific Antibody with Integrated Mass Spectrometry-based Protein Footprinting Approaches**; <u>Richard Huang</u>[1]; Feng Wang[2]; Matthew Wheeler[2]; Bryant Chau[2]; Jia Dong[2]; Winse Morishige[2]; Natalie Bezman[2]; Pavel Strop[2]; Arvind Rajpal[2]; Olafur Gudmundsson[1]; Guodong Chen[1]; [1]*Bristol-Myers Squibb, Princeton, NJ;* [2]*Bristol-Myers Squibb, Redwood City, CA*

TOC am 09:30   **The landscapes of antigen-engaged nanobody proteomes**; <u>Zhe Sang</u>[1]; Yufei Xiang[1]; Dina Schneidman[2]; Yi Shi[1]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*Hebrew University of Jerusalem, Jerusalem, Israel*

TOC am 09:50   **Competitive SEC affinity separation for identification of antibody modifications impacting binding to target protein**; <u>Rachel Liuqing Shi</u>[1]; Gang Xiao[1]; Thomas M Dillon[1]; Arnold Mcauley[1]; Margaret S Ricci[1]; Pavel V. Bondarenko[1]; [1]*Amgen, Inc., Thousand Oaks, CA*

TOC am 10:10   **Deep learning improves sensitivity and specificity of peptide identification in immunopeptidomics**; <u>Kai Li</u>[1, 2]; Bo Wen*[1, 2]; Bing Zhang*[1, 2]; [1]*Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX 77030;* [2]*Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX 77030*

	TOD am: Informatics: Multiomics Integration and Applications
	Chair: Amina Woods (NIDA IRP, NIH)

TOD am 08:30   **Integration of metabolomics & proteomics profiles of NGLY1 deficiency plasma and cellular models to identify molecular phenotypes**; <u>Songjie Chen</u>[1]; Guangwen Wang[1]; Xiaotao Shen[1]; Daniel Hornberg[1]; Michael Snyder[1]; [1]*Stanford University, Stanford, CA*

TOD am 08:50   **DMDB: A database for drug interactions, metabolism and mechanism of action based on integrative Omics**; <u>Raghav Sehgal</u>[1]; Rebecca Cardone[1]; Richard Martyn Williams[1]; Xiaojian Zhao[1]; Qiushi Sun[1]; Surbhi Poddar[2]; Richa Mudgal[2]; Richard Schneider[3]; Richard G. Kibbey[1]; [1]*Yale University, New Haven, CT;* [2]*Elucidata, Delhi, India;* [3]*NIH/NCATS, Rockville, MD*

TOD am 09:10   **Utilizing a Proteogenomic Pipeline to Verify Novel Transcription Events in Neurological Research**; <u>Conor C Jenkins</u>[1, 2]; Benjamin Orsburn[2, 3]; Miranda Darby[1]; [1]*Hood College, Frederick, MD;* [2]*Proteomic Und Genomic Sciences, Glen Rock, PA;* [3]*University of Virginia School of Medicine, Charlottesville, VA*

TOD am 09:30   **Aqueous Humor Metabolite Profile of Pseudoexfoliation Glaucoma is Distinctive**; <u>Ciara Myer</u>[1]; Leila Abdelrahman[1]; Santanu Banerjee[1, 2]; Ram Khattri[3]; Matthew E. Merritt[3]; Anna K. Junk[1, 4]; Richard K. Lee[1]; Sanjoy K. Bhattacharya[1]; [1]*Bascom Palmer Eye Institute, University of Miami, Miami, FL;* [2]*Department of Surgery, University of Miami, Miami, FL;* [3]*University of Florida, Gainesville, FL;* [4]*Miami Veterans Affairs Healthcare System, Miami, FL*

TOD am 09:50   **Automating the Analysis of Multi-Omics Data to Accelerate Breeding and Crop Protection Programs**; <u>Joe Shambaugh</u>[1]; Benjamin J Adamczyk[2]; Thamas Hartsch[3]; Peter Haberl[4]; [1]*Genedata Inc, Lexington, MA;* [2]*Genedata, Lexington, MA;* [3]*Genedata AG, Basel, Switzerland;* [4]*Genedata GmbH, Munich, Germany*

TOD am 10:10   **Advantages of multipronged search and processing tools to analyze TMT-labeled and XL-MS datasets**; Ying Zhang[1]; <u>Zhihui Wen</u>[1]; Michael Washburn[1]; Laurence Florens[1]; [1]*Stowers Institute for Medical Research, Kansas City, MO*

TOE am 08:30   **Tandem MS identifies unexpected components in the ground layer of paintings from the Danish Golden Age**; <u>Fabiana Di Gianvincenzo</u>[1]; Meaghan Mackie[1, 2]; Troels Filtenborg[3]; Cecil Krarup Andersen[3]; Madeleine Ernst[4]; Jørgen Wadum[3]; Enrico Cappellini[1]; *[1]GLOBE institute, University of Copenhagen, Copenhagen, Denmark; [2]Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; [3]National Gallery of Denmark, Copenhagen, Denmark; [4]Center for Newborn Screening, Department of Congenital Disorders, Statens Serum Institut, Copenhagen, Denmark*

TOE am 08:50   **Trace level top down proteomics analysis: application to the study of Gainsborough drawings**; <u>Francesca Galluzzi</u>[1]; Julie Arslanoglu[2]; Catherine Rawlins[1]; Stephane Claverol[1]; Federica Pozzi[2]; Reba F. Snyder[3]; Caroline Tokarski[1]; *[1]Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Proteome Platform, University of Bordeaux, Bordeaux, France; [2]Department of Scientific Research, The Metropolitan Museum of Art, New York, 10028; [3]Thaw Conservation Center, The Morgan Library & Museum, New York, 10016*

TOE am 09:10   **Bioarchaeological Proteomic Analysis of Skin Samples from an Ancient Egyptian Child Mummy**; <u>Prathiba Ravishankar</u>[1]; Dylan Multari[1]; Ronika K Power[1]; Paul A. Haynes[1]; *[1]Macquarie University, North Ryde, Sydney, Australia*

TOE am 09:30   **Large-scale Palaeoproteogenomics to explore the phylogenetic tree of Elephantidae**; <u>Patrick Leopold Ruether</u>[1]; Simon Rasmussen[1]; Immanuel Husic[1]; Marianne Dehasque[2]; Love Dalén[2]; Jesper V Olsen[1]; *[1]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; [2]Center for Palaeogenetics, Stockholm, Sweden*

TOE am 09:50   **Resurrecting the Protein Sequence from Hadrosauridae Egg Shells**; <u>Emily R Sekera</u>[1]; Connor Gould[1]; Nerith Rocio Elejalde Cadena[2]; Abel Moreno Cárcamo[2]; Troy D Wood[1]; *[1]University at Buffalo, Buffalo, NY; [2]Universidad Nacional Autónoma de México, Cayoacán, Mexico*

TOE am 10:10   **GrandPep, a novel software for computational reconstruction of ancient protein sequences**; <u>Petra Gutenbrunner</u>[1]; Frido Welker[2]; Jazmin Ramos-Madrigal[2]; Assa Yeroslaviz[1]; Juergen Cox[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]University of Copenhagen, Evolutionary Genomics Section, Globe Institute, Copenhagen, Denmark*

TOF am 08:30   **A novel straightforward in vivo cross-linking mass spectrometry strategy for proteome-wide studies**; <u>Lucienne Nouchikian</u>[1]; Martial Rey[1]; Jonathan Dhenin[1]; Youxin Kong[1]; Guillaume Duménil[1]; Julia Chamot-Rooke[1]; *[1]Institut Pasteur, Paris, France*

TOF am 08:50   **A combination of top-down and cross-linking mass spectrometry illuminates the pairing of PSII-LHCII supercomplexes across thylakoid membranes**; Pascal Albanese[1, 2, 3]; Sem Tamara[3, 4]; Cristina Pagliano[1]; <u>Richard Scheltema</u>[3, 4]; *[1]Applied Science and Technology Department–BioSolar Lab, Politecnico di Torino, Torino, Italy; [2]Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; [3]Netherlands Proteomics Center, Utrecht, Netherlands; [4]Biomolecular Mass Spectrometry and Proteomics, Utrecht Institute for pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands*

TOF am 09:10   **In-depth characterisation of UV-induced cross-linking in a model protein-RNA complex: Implications for structural proteomics of ribonucleoproteins**; <u>Chris P. Sarnowski</u>[1]; Anna Knörlein[2]; Tebbe De Vries[3]; Michael Götze[1]; Ruedi Aebersold[1, 4]; Frédéric H-T Allain[3]; Jonathan Hall[2]; Alexander Leitner[1]; *[1]Institute of Molecular Systems Biology, Department of Biology, ETH Zürich, Zürich, Switzerland; [2]Institute of Pharmaceutical Sciences, Department of Chemistry, ETH Zürich, Zürich, Switzerland; [3]Institute of Biochemistry, Department of Biology, ETH Zürich, Zurich, Switzerland; [4]Faculty of Science, University of Zürich, Zurich, Switzerland*

TOF am 09:30   **Stitching the synapse: untargeted cross-linking mass spectrometry (XL-MS) into resolving synaptic protein interactions**; <u>Miguel A Gonzalez-Lozano</u>[1]; Frank Koopmans[1]; Patrick F Sullivan[2]; Jonas Protze[3]; Gerd Krause[3]; Matthijs Verhage[1]; Ka Wan Li[1]; Fan Liu[3]; August B Smit[1]; *[1]Vrije University Amsterdam, Amsterdam, Netherlands; [2]Karolinska Institutet, Stockholm, Sweden; [3]Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany*

TOF am 09:50   **Using In-Cell Fast Photochemical Oxidation of Proteins to Observe Changes in Gleevec's Drug Target Engagement in Triple Negative Breast Cancer**; Emily E Chea[1]; <u>Lisa Jones</u>[2]; *[1]University of Maryland Balitmore, Baltimore, MD; [2]University of Maryland, Baltimore, MD*

TOF am 10:10   **First Draft of the Human Lysosomal Interactome by Cross-Linking Mass Spectrometry Reveals Novel Interactions and Structures**; <u>Jasjot Singh</u>[1]; Hadeer Elhabashy[2]; Volkmar Gieselmann[1]; Oliver Kohlbacher[2]; Dominic Winter[3]; *[1]Institute of Biochemistry and Molecular Biology - University Bonn, Bonn, Germany; [2]Institute*

for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]Institute of Biochemistry and Molecular Biology - University Bonn, Bonn, Germany

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TOG am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements

Chair: Ann Knolhoff (FDA)

TOG am 08:30 **Inhibitory mechanism and kinetics of active components of licorice Glycyrrhiza uralensisFisch. ex DC. on human cytochrome P450 enzymes**; Luying Chen[1, 2]; Laura Tyler[2]; Dejan S. Nikolic[2]; Guannan Li[2]; Guido F. Pauli[2]; Richard B. van Breemen[1, 2]; *[1]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; [2]UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL*

TOG am 08:50 **Development of MS-based detection method for cashew proteins in an oil matrix based on a comprehensive protein database**; Shimin Chen[1]; Melanie Downs[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE*

TOG am 09:10 **Liquid is better: liquid AP-MALDI MS high-throughput analysis for food adulterations, diagnostics and early animal disease detection**; Cristian Piras[1]; Barney Jones[2]; Nick Taylor[2]; Oliver J Hale[1]; Michael Morris[3]; Chris Reynolds[2]; Rainer Cramer[1]; *[1]Department of Chemistry, University of Reading, Reading, United Kingdom; [2]Centre for Dairy Research (CEDAR), School of Agriculture, Policy and Development, University of Reading, Reading, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

TOG am 09:30 **Automated chiral analysis of free amino acids in fermented foods by trapped ion mobility-mass spectrometry**; Jonas M. Will[1]; Arne Behrens[1]; Marcel Macke[1]; C. Derrick Quarles Jr. [2]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; [2]Elemental Scientific, Inc. (ESI), Omaha, Nebraska*

TOG am 09:50 **Integrating Metabolomics and NIR Spectral Data for Fruit Quality Assessment and Their Applications in Apple Breeding**; Kevin Hooton[1]; Rachael Leblanc[1]; David Liscombe[1]; *[1]Vineland Research and Innovation Centre, Vineland Station, Ontario*

TOG am 10:10 **Empty Slot.** Stay tuned for promoted selection to be made.

TOH am: Homeland Security, Defense, and Extreme Environments: Developments and Applications

Chair: Trevor Glaros (CCDC Chemical Biological Center)

TOH am 08:30 **Quantitative proteomic-based approaches development to study the human proteome changes during real space missions and ground-based experiments**; Alexey Kononikhin[1, 2]; Alexander Brzhozovskiy[1, 2]; Anna Bugrova[3]; Maria Indeykina[3]; Daria Kashirina[2]; Anna Ryabokon[3]; Ludmila Pastushkova[2]; Igor Popov[4]; Irina Larina[2]; Christoph H. Borchers[1, 5]; Eugene (evgeny) Nikolaev[1]; *[1]Skolkovo Institute of Science and Technology, Moscow, Russia; [2]Institute of Biomedical Problems, Russian Academy of Sciences, Moscow, Russia; [3]Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow,, Russia; [4]Moscow Institute of Physics and Technology, Dolgoprudny, Russia; [5]McGill University, Montreal, QC*

TOH am 08:50 **Combination of Surface-Enhanced Raman Spectroscopy and Paper Spray Ionization on Portable Instrumentation for On-Site Drug Analysis**; Ashley Stelmack[1]; Christopher C. Mulligan[1]; William L. Fatigante[1]; Daniel S. Burr[1]; Noah W. McClurg[1]; Trevor J. McDaniel[1]; Jemima Lartey[1]; Jamie R. Wieland[1]; Jeremy D. Driskell[1]; Jun-Hyun Kim[1]; *[1]Illinois State University, Normal, IL*

TOH am 09:10 **Development of a drone-based TF-SPME water sampler for the on-site screening of environmental pollutants and protection at remote locations**; Jonathan J Grandy[1]; Virginia Galpin[2]; Varoon Singh[2]; Janusz Pawliszyn[1]; *[1]Univeristy of Waterloo, Waterloo, ON; [2]University of Waterloo, Waterloo, ON*

TOH am 09:30 **Identification of Diagnostic Markers Indicative of Exposure to Energetic Materials Using Mass Spectrometric Techniques and Random Forest Classification**; Cameron Longo[1]; Samira Beyramysoltan[1]; Rabi A. Musah[1]; *[1]University at Albany - SUNY, Albany, NY*

TOH am 09:50 **The Advantages of Two-Dimensional Mass Spectrometry Analysis of Agrochemicals in Environmental Samples**; Bryan P. Marzullo[1]; Tomos E. Morgan[1]; Christopher A. Wootton[1]; Simon J. Perry[2]; Mansoor Saeed[2]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]SYNGENTA, Bracknell, United Kingdom*

TOH am 10:10 **On-demand Atmospheric Arc Ionization for Analyzing Swabbed Samples Using Miniature Mass Spectrometer**; Ningxi Li[1]; Zhijun Cai[1]; Wenbo Cao[1]; Huarong Gu[1]; Zheng Ouyang[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China*

TOA pm: Instrumentation: Portable and Transportable Mass Spectrometers

Chair: Donna Hollinshead

TOA pm 02:30   **Intelligent Handheld Mass Spectrometer for On-Site Analysis**; <u>Bin Jiao</u>[1]; Xinwei Liu[1]; Jiexun Bu[2]; Huimin Ye[1]; Zheng Ouyang[1]; [1]*Tsinghua University, Beijing, China;* [2]*PURSPEC Technologies, Beijing, China*

TOA pm 02:50   **2D MS/MS Scans on Benchtop and Portable Ion Trap Mass Spectrometers**; <u>Lucas Szalwinski</u>[1]; Dylan T Holden[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN*

TOA pm 03:10   **Measurement of THC in Exhaled Breath after Marijuana smoking: Exploring The Potential of a Transportable LC-CMS System**; Olof Beck[1]; <u>Jack Henion</u>[2]; Sabina Seferaj[3]; Peter Stambeck[4]; [1]*Department of Clinical Neurosciences, Stockholm, Sweden;* [2]*Advion Inc., Ithaca, NY;* [3]*Karolinska University Hospital, Stockholm, Sweden;* [4]*Munkplast AB, Uppsala, Sweden*

TOA pm 03:30   **Design considerations for a cycloidal mass analyzer**; <u>Elettra L. Piacentino</u>[1]; Kathleen Horvath[1]; Maria Luisa Sartorelli[2]; Tanouir Aloui[3]; Raul Vyas[1]; Rafael Bento Serpa[1]; Charles B. Parker[1]; Yuriy Zhilichev[4]; Roger P Sperline[5]; Robert Kingston[5]; Scott Tilden[6]; Justin Keogh[5]; Jeffrey T Glass[1]; Jason J Amsden[1]; M. Bonner Denton[5]; [1]*Duke University, Durham;* [2]*Universidade Federal de Santa Catarina, Trindade, Brazil;* [3]*Duke University, Durham, North Carolina;* [4]*Consultant, Durham, North Carolina;* [5]*University of Arizona, Tucson, AZ;* [6]*University of Arizona, Tucson, AZ 85351*

TOA pm 03:50   **Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer: End-to-End Testing, Performance, and Integrated Operations Demonstration**; <u>Ryan M. Danell</u>[1, 2]; Andrej Grubisic[1]; Desmond Kaplan[1, 3]; Friso H.w. Van Amerom[1, 4]; Xiang Li[1, 5]; Marco E Castillo[1, 6]; Caroline Freissinet[7]; Arnaud Buch[8]; Melissa Guzman[7]; Fabien Stalport[9]; Noel Grand[9]; Cyril Szopa[7, 10]; Walter Goetz[11]; Stephanie A Getty[1]; François Raulin[9]; William B Brinckerhoff[1]; Fred Goesmann[11]; [1]*NASA Goddard Space Flight Center, Greenbelt, MD;* [2]*Danell Consulting, Inc., Winterville, NC;* [3]*KapScience LLC, TEWKSBURY, MA;* [4]*Mini-Mass Consulting, Inc., Hyattsville, MD;* [5]*University of Maryland Baltimore County, Baltimore, MD;* [6]*ATA Aerospace, Greenbelt, MD;* [7]*LATMOS/IPSL University of Versailles-Saint-Quentin-en-Yvelines, Guyancourt, France;* [8]*CentraleSupélec, Paris, France;* [9]*LISA, U. Paris-Est, Créteil, U. Paris Diderot, Paris, France;* [10]*Institut Universitaire de France, Paris, France;* [11]*Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany*

TOA pm 04:10   **Dragonfly Mass Spectrometer Boldly Goes Where No Other Ion Trap Mass Spectrometer Has Gone Before: Saturn's Moon Titan**; <u>Andrej Grubisic</u>[1]; Melissa G. Trainer[2]; William B. Brinckerhoff[2]; Friso H. W. Van Amerom[2, 3]; Xiang Li[2, 4]; Ryan M. Danell[2, 5]; Desmond Kaplan[2, 6]; Charles A. Malespin[2]; John T. Costa[7]; Fredrik Rehnmark[7]; Kris Zacny[7]; Ralph D. Lorenz[8]; Jason W. Barnes[9]; Elizabeth P. Turtle[8]; [1]*NASA, Greenbelt, MD;* [2]*NASA Goddard Space Flight Center, Greenbelt, MD;* [3]*Mini-Mass Consulting, Inc., Hyattsville, MD;* [4]*University of Maryland Baltimore County, Baltimore, MD;* [5]*Danell Consulting, Inc., Winterville, NC;* [6]*KapScience LLC, TEWKSBURY, MA;* [7]*Honeybee Robotics, Altadena, CA;* [8]*Johns Hopkins University Applied Physics Laboratory, Laurel, MD;* [9]*University of Idaho, Moscow, ID*

TOB pm: Lipidomics: Targeted and Untargeted

Chair: Michelle Reid (ETH Zurich)

TOB pm 02:30   **LipidXplorer 2.0 Web: Online tool for simplified and streamlined lipid identification, visualization and quantification by shotgun lipidomics**; <u>Eduardo Jacobo Miranda Ackerman</u>[1]; Nils Hoffmann[2]; Oskar Knittelfelder[1]; Kai Schuhmann[1]; Olga Vvedenskaya[1]; Andrej Shevchenko[1]; [1]*Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany;* [2]*Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

TOB pm 02:50   **A Lipid Analysis Pipeline for Mapping Lipid Transducers of Exercise in Rats**; <u>David Gaul</u>[1]; Sam Moore[1]; Alexandra Coomes[2]; Karyn A. Esser[2]; Brent G. Alberston[3]; Michael F. Hirshman[3]; Laurie J. Goodyear[3]; Facundo M. Fernandez[1]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*University of Florida, Gainesville, FL;* [3]*Harvard Medical School, Boston, MA*

TOB pm 03:10   **Lipidomic analysis of an SCD inhibitor that reduces α-synuclein neurotoxicity**; <u>Xiaoping L Hronowski</u>[1]; Stanley Goldstein[1]; Junmin Wang[1]; Ru Wei[1]; Andreas Weihofen[1]; Silke Nuber[2]; Dennis Selkoe[2]; [1]*Biogen, Inc., Cambridge, Massachusetts;* [2]*Brigham and Women's Hospital, Harvard Medical School, Boston, Massachusetts*

TOB pm 03:30   **Mass spectrometry analysis reveals altered fatty acid levels in the brain of the symptomatic Niemann-Pick, type C1 mouse model**; <u>Melissa R. Pergande</u>[1]; Koralege C. Pathmasiri; Thu T.A. Nguyen[1]; Stephanie M. Cologna[1]; [1]*University of Illinois at Chicago, Chicago, IL*

TOB pm 03:50   **Broad Lipid Coverage and Cellular-Level MALDI-Imaging of Lipids Using Oversampling Combined with Laser Post-Ionization**; <u>Shane R. Ellis</u>[1, 2]; Andrew P. Bowman[2]; Jeroen F. J. Bogie[3]; Jerome J. A. Hendriks[3]; Mansour Haidar[3]; Mikhail Belov[4]; Ron M.A Heeren[2]; [1]*Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia;* [2]*Maastricht MultiModal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Limburg, Netherlands, Maastricht, Netherlands;*

[3]*Department of Immunology and Infection, Biomedical Research Institute, Hasselt University, Hasselt, Belgium; [4]Spectroglyph LLC, Kennewick, Washington*

TOB pm 04:10 **Following de novo triglyceride dynamics using stable isotope LC-FT-ICR MS/MS**; <u>Lilian Tose</u>[1]; Chad R. Weisbrod[2]; Francisco A. Fernandez-Lima[1]; [1]*Florida International University, Miami, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL*

TOC pm: Biomarkers: Qualitative Analysis
Chair: Melissa Carter (CDC)

TOC pm 02:30 **Linking Brain Tissue Lipid Distributions and Serum Biomarkers of Traumatic Brain Injury**; <u>Eric C. Gier</u>[1]; Clint M. Alfaro[1]; Alexis N. Pulliam[2]; David A. Gaul[1]; Samuel G. Moore[1]; Michelle C. Laplaca[2]; Facundo M. Fernandez[1]; [1]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, 30332; [2]Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, Georgia*

TOC pm 02:50 **Profiling RNA Modifications in Central Nervous Tissue by Mass Spectrometry Reveals Spatiotemporal Heterogeneity in the Neural Epitranscriptome during Non-Associative Learning**; <u>Kevin Clark</u>[1]; Yanqi Tan[2]; Jonathan V Sweedler[1, 2]; [1]*Beckman Institute, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

TOC pm 03:10 **Cell and Proteoform-Specific Top-Down Proteomics Reveals Biomarkers of Acute Liver Rejection**; <u>Paul M Thomas</u>[1]; Robert V Gerbasi[1]; Rafael D Melani[1]; Ryan T Fellers[1]; Joseph B Greer[1]; Richard D Leduc[1]; Timothy K. Toby[1]; Joshua Levitsky[2]; Neil L Kelleher[1]; [1]*Northwestern University, Evanston, IL; [2]Northwestern University, Chicago, IL*

TOC pm 03:30 **Spatially-Targeted Proteomics for Analysis of Host-Pathogen Interactions in Staphylococcus aureus**; <u>Emma R Guiberson</u>[1, 2]; Daniel J Ryan[1, 2]; Andy Weiss[3]; Eric P Skaar[3]; Richard M. Caprioli[1, 2, 4, 5, 6]; Jeffrey M. Spraggins[1, 2, 4]; [1]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Medicine, Vanderbilt University, Nashville, TN; [6]Department of Pharmacology, Vanderbilt University, Nashville, TN*

TOC pm 03:50 **Equine Biological Passport using Orbitrap Exploris 480**; <u>Sophie Bromilow</u>[1]; Claudia P.B. Martins[2]; Amanda Lee[2]; Michael W. Senko[2]; Scott D Stanley[1]; [1]*University of Kentucky, Lexington, KY; [2]ThermoFisher Scientific, San Jose, CA*

TOC pm 04:10 **Targeted and Untargeted Metabolomics for Monitoring and Assessing Soldier Tactical Readiness and Effectiveness**; <u>Elizabeth S Dhummakupt</u>[1]; Richard Lawrence[1]; Ethan Mcbride[1]; Philliip Mach[1]; Conor Jenkins[2]; Trevor Glaros[1]; Erika Hussey[3]; John Ramsay[3]; [1]*CCDC-Chemical Biological Center, APG-EA, MD; [2]Excet, Inc., Springfield, VA; [3]CCDC-Soldier Center, Natick, MA*

TOD pm: Imaging: Instrumentation & Method Development
Chair: Isabelle Fournier (University of Lille)

TOD pm 02:30 **Improvements in Ionisation to Improve Relative Quantitation in Secondary Ion Mass Spectrometry (SIMS) of biosamples using Water Cluster Ion Beams**; Kelly Dimovska Nilsson[1]; Anthi Karagianni[1]; <u>John Fletcher</u>[1]; [1]*University of Gothenburg, Gothenburg, Sweden*

TOD pm 02:50 **Mass Spectrometry Imaging of Biopolymers in Infected Plant Tissues by Laser Desorption Ionization from Silicon Nanopost Arrays**; <u>Laith Samarah</u>[1]; Tina H Tran[1]; Gary Stacey[2]; Akos Vertes[1]; [1]*The George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO*

TOD pm 03:10 **Isomer-resolved imaging of phospholipids using nano-DESI coupled with on-line photochemical reaction with singlet oxygen**; <u>Daisy M Unsihuay Vila</u>[1]; Pei Su[1]; Xiaofei Sun[2]; Sudhansu K Dey[2]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

TOD pm 03:30 **Chemical Decrosslinking of Analytes in Formaldehyde-Fixed Paraffin-Embedded Pancreas for Mass Spectrometry Imaging**; <u>Dongkyu Lee</u>[1]; Stanislav S. Rubakhin[1, 2]; Jonathan V Sweedler[1, 2]; [1]*Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL; [2]Beckman Institute, Urbana, IL*

TOD pm 03:50 **Developments in native mass spectrometry imaging with liquid extraction surface analysis**; <u>Oliver J Hale</u>[1]; Helen J Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

TOD pm 04:10 **Ambient mass spectrometry imaging of biological tissue with atmospheric pressure UV-laser desorption low temperature plasma post-ionization**; <u>Bin Yan</u>[1]; Rory T Steven[1]; Teresa Murta[1]; Efstathios A Elia[1]; Marcel Niehaus[1]; Kenneth N Robinson[1]; Martin Metodiev[1, 2]; Josephine Bunch[1, 2]; [1]*National Physical Laboratory, Teddington, United Kingdom; [2]Imperial College London, London, United Kingdom*

	TOE pm: Cannabis Testing
	Chair: Brigitte Simons (Pasha Brands)

TOE pm 02:30 **Cannabinoidomics – An Analytical Tool to Understand the Effect of Medical Cannabis Treatment in Clinical and Preclinical Studies**; Paula Berman[1]; Liron Sulimani[2]; Anat Gelfand[1]; Keren Amsalem[1]; Gil M Lewitus[1]; David Meiri[1]; [1]*Technion - Israel Institute of Technology, Haifa, Israel;* [2]*Cannasoul Analytics, Caesarea, Israel*

TOE pm 02:50 **Investigation of Tetrahydrocannabinol (Δ9-THC) and Cannabidiol (CBD) in Smoke by Application of an On-Line Photo Ionization Mass Spectrometry**; Sven Ehlert[1, 2]; Jan Heide[2]; Andreas Walte[1]; Ralf Zimmermann[2, 3]; [1]*Photonion GmbH, Schwerin, Germany;* [2]*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany;* [3]*Heltmholtz Center, Munich, Germany*

TOE pm 03:10 **Vaping-Related Outbreak: Unique Information from Direct Analysis in Real-Time Mass Spectrometry**; Travis M. Falconer[1]; Adam C. Lanzarotta[1]; Robert A. Wilson[1]; Rick A. Flurer[1]; [1]*US Food & Drug Administration, Cincinnati, OH*

TOE pm 03:30 **Characterizing Products Intended for Inhalation After High-Temperature Vaporization**; Nahanni Sagar[1]; Seamus Riordan-Short[1]; Rob O'brien[1, 2]; Matthew Noestheden[1, 2]; [1]*Supra R&D, Kelowna, BC;* [2]*University of British Columbia, Kelowna, BC*

TOE pm 03:50 **Characterization of Beverage Products containing Cannabidiol (CBD) by GC-MS and GCxGC-MS**; Elizabeth Humston-Fulmer[1]; Christina Kelly[1]; David E Alonso[1]; Joe Binkley[1]; Lorne Fell[1]; [1]*LECO Corporation, Saint Joseph, MI*

TOE pm 04:10 **A Robust LC-QQQ Method for the Analysis of Pesticides and Mycotoxins in Cannabis Samples According to Health Canada Regulations**; Hanieh Peyman[1]; Heather Gamble[1]; Kaveh Kahen[1]; [1]*Sigma Analytical, Scarborough, ON*

	TOF pm: Nucleic Acids and Oligonucleotides
	Chair: Amber Mosley (Indiana University)

TOF pm 02:30 **Revealing molecular detail of DNA triplexes to underpin antigene technology**; Alexander Begbie[1]; Jack Klose[1]; Jiawei Li[1]; Tara L Pukala[1]; [1]*University of Adelaide, Adelaide, Australia*

TOF pm 02:50 **Ribonucleic Acid Sequence Characterization by Activated Ion-Negative Electron Transfer Dissociation (AI-NETD) Mass Spectrometry**; Trenton M Peters-Clarke[1]; Qiuwen Quan[1]; Dain R Brademan[1]; Alexander S Hebert[1]; Michael S Westphall[1]; Joshua J Coon[1]; [1]*University of Wisconsin-Madison, Madison, WI*

TOF pm 03:10 **Hybridization LC-MS/MS: An Alternative Bioanalytical Method for Anti-Sense Oligonucleotide Quantitation in Plasma and Tissue Samples**; Pei Li[1]; Yuqing Gong[1]; Jaeah Kim[2]; Jp Gilbert[1]; Hannah Certo[1]; Rachel Groth[1]; Michael Rooney[1]; [1]*Biogen, Cambridge, MA;* [2]*Atrium Staffing, Boston, MA*

TOF pm 03:30 **Database Search of Tandem Mass Spectra of Oligonucleotides**; Marshall W. Bern[1]; Rose D Lawler[1]; Wilfred Tang[1]; Eric Carlson[1]; Maria Basanta-Sanchez[1]; Ines C Santos[2]; Jennifer S Brodbelt[2]; [1]*Protein Metrics Inc., Cupertino, CA;* [2]*University of Texas at Austin, Austin, TX*

TOF pm 03:50 **Novel aspects of augmenting protein–nucleic acid cross-link identification by high-field asymmetric-waveform ion-mobility mass spectrometry (FAIMS)**; Alexander Wulf[1]; Rosa Viner[2]; Timo Sachsenberg[3]; Oliver Kohlbacher[3]; Henning Urlaub[4, 5]; [1]*Max Planck Institute for biophysical chemistry, Göttingen, Germany;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Center for Bioinformatics, University of Thübingen, Thübingen, Germany;* [4]*Max Planck Institute for biophysical chemistry, Göttingen, Germany;* [5]*Bioanalytics Group, University Medical Center Göttingen (UMG), Göttingen, Germany*

TOF pm 04:10 **On-line capillary electrophoresis-UVPD-mass spectrometry for the characterization of nucleic acids**; Ines C Santos[1]; Jada N. Walker[1]; Marshall Bern[2]; Maria Basanta-Sanchez[2]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*Protein Metrics Inc., Cupertino, CA*

	TOG pm: Glycopeptides and Glycoproteins
	Chair: Lingjun Li (University of Wisconsin)

TOG pm 02:30 **Effective MS-Based Chemical Methods for Comprehensive Analysis of Glycoproteins**; Ronghu Wu[1]; Fangxu Sun[1]; [1]*Georgia Institute of Technology, Atlanta, GA*

TOG pm 02:50 **Enhanced N-sialoglycoproteomic Profile by Using Zwitter-Ionic Hydrophilic Interaction Chromatography (ZIC-cHILIC)**; Yi-Ju Chen[1]; Ta-Chi Yen[1]; Yu-Hsien Lin[1]; Kai-Hooi Khoo[2]; Yu-Ju Chen[1]; [1]*Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*

TOG pm 03:10 **Comprehensive N- and O-Glycoproteomics with MSFragger Mass Offset Search**; Daniel A. Polasky[1]; Fengchao Yu[1]; Guo Ci Teo[1]; Felipe Da Veiga Leprevost[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

TOG pm 03:30 **Multi-Glycomic Platform for Mapping the Human Brain Glycocalyx in Alzheimer's Disease Patients in a Region-Specific Manner using nanoLC-MS Methods**; Jennyfer Tena[1]; Mariana Barboza[1]; Maurice Wong[1]; Carlito B Lebrilla[1]; [1]*UC Davis, Davis, CA*

TOG pm 03:50 **How unique is our plasma proteome? Answers from top-down native mass spectrometry**; Albert J.R. Heck; *Utrecht University, Utrecht, Netherlands*

TOG pm 04:10 **Multiplexed Imaging Mass Spectrometry of the Extracellular Matrisome using Serial Enzyme Digests from Formalin-Fixed Paraffin Embedded Tissue Sections**; Cassandra L Clift[1]; Anand Mehta[1]; Richard R Drake[1]; Peggi M Angel[1]; [1]*Medical University of South Carolina, Charleston, SC*

	TOH pm: Fundamentals: Native MS
	Chair: Saiful Chowdhury (Univerisity of Texas at Arlington)

TOH pm 02:30 **Design and application of an alpha particle electrospray source for native mass spectrometry analysis of theoretically unresolvable glycoprotein therapeutic targets**; Elizabeth Hecht[1]; Ben Aguilar[2]; Ananya Dubey[2]; Wendy Sandoval[1]; Henry Benner[2]; [1]*Genentech Inc., South San Francisco, CA; [2]Ion Dx, Monterey, CA*

TOH pm 02:50 **Statistical Analysis of Ultraviolet Photodissociation of Native-Like Proteins**; Luis A Macias[1]; Jennifer Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

TOH pm 03:10 **Trends and applications from >10,000 fragment ions produced by higher-energy collisional dissociation of 159 native monomers and 70 native complexes**; Ashley N Ives[1]; Taojunfeng Su[1]; Kenneth R Durbin[1, 2]; Bryan P Early[1]; Henrique dos Santos Seckler[1]; Ryan T Fellers[1, 2]; Richard D Leduc[1]; Luis F Schachner[1]; Steve M Patrie[1]; Neil L Kelleher[1]; [1]*Northwestern University, Evanston, IL/60208; [2]Proteinaceous, Evanston, IL*

TOH pm 03:30 **Combining native mass spectrometry with mass photometry to quantify ultra-heterogeneous protein assemblies**; Miranda P Collier[1]; Dominik Saman[1]; Justin LP Benesch[1]; [1]*University of Oxford, Oxford, United Kingdom*

TOH pm 03:50 **Electrospray Surface Charge Describes Protein Molecular Motion**; Rod Chalk[1]; Oktawia Borokowska[1, 2]; Petra Born[3]; Ole Tietz[1]; Opher Gileadi[1]; Nicola Burgess-Brown[1]; [1]*Oxford University, Oxford, United Kingdom; [2]Lonza, Slough, United Kingdom; [3]Max Plank Institute, Dresden, Germany*

TOH pm 04:10 **Improving mass measurements of protein complexes through IR activation coupled with charge reduction ion/ion reactions**; Kenneth W. Lee[1]; Christopher P. Harrilal[1]; Liangxuan Fu[1]; Gregory S. Eakins[1]; Scott A. Mcluckey[1]; [1]*Purdue University, West Lafayette, IN*

WOA am: Instrumentation: Innovative Separations Approaches Coupled to MS
Chair: Honglan Shi (Missouri University)

WOA am 08:30   **Qualitative and quantitative advantages of Liquid Electron Ionization (LEI) interface in pesticides analysis of complex matrices**; Veronica Termopoli[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Mansoor Saeed[3]; Simon J. Perry[3]; Pablo Navarro[3]; Helene Fain[3]; Achille Cappiello[1, 2]; *[1]University of Urbino, Urbino, Italy; [2]Vancouver Island University, Nanaimo, BC; [3]SYNGENTA, Bracknell, United Kingdom*

WOA am 08:50   **New Double Barrel ESI Source and Novel Tandem NanoLC-MS Setup Enables 24/7 Proteome Profiling and Close to 100% MS Utilization**; Runsheng Zheng[1]; Thomas Lanzinner[2]; Georg Völkle[3]; Christopher Pynn[4]; Jan Linnemann[2]; John Modrow[2]; Wim Decrop[4]; Andreas Tebbe[2]; Peter Jehle[4]; Oleksandr Boychenko[4]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Evotec (München) GmbH, Martinsried, Germany; [3]Sonation GmbH, Biberach, Germany; [4]Thermo Fisher Scientific, Germering, Germany*

WOA am 09:10   **Native Ion-Mobility Coupled to a Q Exactive UHMR Orbitrap MS: Protein Complexes at Ultra High Resolution**; Jacob W. McCabe[1]; Christopher S. Mallis[1]; Klaudia I. Kocurek[1]; Joanna K. Denton[1]; John M. Gordon[1]; Mehdi Shirzadeh[1]; Michael L. Poltash[1]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

WOA am 09:30   **A Liquid-phase Ion Trap for Ion Trapping, Transfer and Sequential Ejection in Solutions**; Jie Hong; *Beijing Institute of Techonology, Beijing, China*

WOA am 09:50   **A Novel Nanoflow ESI Probe Optimized for Emitters with Chromatographic Packing**; Yang Kang[1]; Leigh Bedford[1]; Stanislaw Potyrala[1]; Bradley B. Schneider[1]; *[1]SCIEX, Concord, ON*

WOA am 10:10   **Towards Online Single Cellular Metabolomics from a Cell Suspension Using Electrospray**; Catherine Munteanu[1]; Shahd Abuhelal[1]; Chelsea Nikula[1]; Daniel Simon[1]; David Gaboriau[1]; Andreas Dannhorn[3]; Efstathios Elia[2]; Richard Goodwin[3]; Josephine Bunch[2, 4]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom; [2]National Physical Laboratory, Teddington, United Kingdom; [3]AstraZeneca, BioPharmaceuticals R&D, Imaging and AI, Clinical Pharmacology and Safety Sciences, Cambridge, United Kingdom; [4]Imperial College London, London, United Kingdom*

WOB am: Cancer Research
Chair: Jurre Kamphorst (Rheos Medicines Inc.)

WOB am 08:30   **Quantitative Proteomics of the Cancer Cell Line Encyclopedia**; David Nusinow[1]; John Szpyt[2]; Steven P Gygi[2]; *[1]Harvard Medical School, Boston, MA; [2]Harvard Medical School, boston, MA*

WOB am 08:50   **Multi-omic discovery of metabolic rewiring in triple-negative breast cancer following mitochondrial folate transport ablation**; Qiuying Chen[1]; Joshua B. Zuk[1]; Christine A. Miller[2]; Steve M. Fischer[2]; Steven S. Gross[1]; *[1]Weill Cornell Medicine, New York, NY; [2]Agilent Technologies, Santa Clara, CA*

WOB am 09:10   **Mass Spectrometry Imaging of N-Glycan Profiles in Tissue Microarrays of Metastatic Breast Cancer Patients Reveals Glycosylation Patterns in Metastasis**; Klara Scupakova[1]; Oluwatobi Adelaja[2]; Benjamin Balluff[1]; Caitlin M. Tressler[2]; Pedram Argani[2]; Ron M.A Heeren[1]; Kristine Glunde[2, 3]; *[1]Maastricht Multimodal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; [2]Johns Hopkins School of Medicine, Baltimore, Maryland; [3]Sidney Kimmel Comprehensive Cancer Center, Baltimore, Maryland*

WOB am 09:30   **Recombinant MHC class I protein with isotope coded peptides enables relative and absolute quantification of the immunopeptidome**; Lauren E Stopfer[1, 2]; Joshua M Mesfin[2]; Brian A Joughin[1, 2]; Douglas A Lauffenburger[1, 2]; Forest M White[1, 2]; *[1]Koch Institute for Integrative Cancer Research, Cambridge, MA; [2]Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA*

WOB am 09:50   **Streamlined Proteomic Profiling of quantity-limited Clinical Tissue facilitated by automated Sample Preparation and Mass Spectrometry**; Torsten Mueller[1]; Mathias Kalxdorf[1, 2]; Romano Hebeler[3]; Scarlet Koch[3]; Marcel Kool[1, 4]; Kristian Pajtler[1, 4]; Jeroen Krijgsveld[1]; *[1]DKFZ, Heidelberg, Germany; [2]EMBL - European Molecular Biology Laboratory, Heidelberg, Germany; [3]Bruker Daltonics, Bremen, Germany; [4]KiTZ - Hopp Children's Cancer Center, Heidelberg, Germany*

WOB am 10:10   **Determining the Origins of Fumarate Accumulation in Patient-Derived Fumarate Hydratase-Deficient Tumor Cell Lines**; Daniel Crooks[1]; Nunziata Maio[2]; Ye Yang[1]; Youfeng Yang[1]; Bhargav Arimilli[3]; Ramon Sun[4]; Tracey Rouault[2]; Richard Higashi[4]; Teresa Fan[4]; Andrew Lane[4]; W. Marston Linehan[1]; Penghui Lin[4]; *[1]National Cancer Institute, Bethesda, MD; [2]Eunice Kennedy Shriver NICHD, National Institutes of Health, Bethesda, Maryland; [3]UT Southwestern Medical Center, Dallas, TX; [4]University of Kentucky, Lexington, KY*

WOC am: Drug Target Identification by MS

Chair: Silvi Chacko (Bristol-Myers Squibb)

WOC am 08:30 **Automated data analysis workflow for high throughput compound screening using Bruker MALDI-TOF platform**; Serhiy Hnatyshyn[1]; Jingjing Deng[1]; Joseph Scavetta[2]; Rostyslav Hnatyshyn[2]; David Harden[1]; *[1]BMS Co., Princeton, NJ; [2]Rowan University, Glassboro, NJ 08028*

WOC am 08:50 **Label-free target identification in one-pot 2D format: evaluation and method comparison using a broad-spectrum kinase inhibitor**; Yingrong Xu[1]; Graham M. West[1]; Mario Abdelmessih[1]; Robert A. Everley[1]; *[1]Pfizer Worldwide Research and Development, Groton, CT*

WOC am 09:10 **Kinase specificity characterization of a PROTAC directed against BRAFV600E**; Ganna Posternak[1, 2]; Xiaojing Tang[1]; Pierre Maisonneuve[1]; Ting Jin[3]; Hugo Lavoie[3]; Zhe Yin[1, 4]; Ahmed Aman[2]; Michael Prakesch[2]; Gennady Poda[2]; Cassandra Wong[1]; Stefan Maier[1]; Julia Kitaygorodsky[1, 4]; Brett Larsen[1]; Karen Colwill[1]; Robert Batey[4]; Mikko Taipale[4, 5]; Igor Kourinov[6]; David Uehling[2]; Anne-Claude Gingras[1, 4]; Rima Al-Awar[2]; Marc Therrien[3]; Frank Sicheri[1, 4]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto; [2]Ontario Institute for Cancer Research, Toronto, ON; [3]University of Montreal, Montreal, QC; [4]University of Toronto, Toronto, ON; [5]Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; [6]NE-CAT, Argonne, IL*

WOC am 09:30 **Quantitative proteomics identifies novel substrates of pomalidomide**; Raghothama Chaerkady[1]; Saghar Nourian[1]; Hsiang-En Hsu[1]; Nazzareno Dimasi[1]; Sonja Hess[1]; *[1]AstraZeneca R&D, Gaithersburg, MD*

WOC am 09:50 **An Integrative Genomics, Metabolomics and Lipidomics Approach to Identify and Validate New Pharmaceutical Drug Targets**; Silvia Aldi[1]; Gregory Hamm[2]; Ljubica Matic[3]; Danielle Van Keulen[4]; Dennie Tempel[4]; Kim Holmstrøm[5]; Boye Schnack[5]; Valur Emilsson[6]; Mariette Lengquist[3]; Per Eriksson[3]; David Bonnel[2]; Alain J Gool[7]; Jonathan Stauber[8]; Ulf Hedin[3]; Eva Hurt Camejo[9]; *[1]Karolinska Institute, Solna, Sweden; [2]ImaBiotech, Loos, France; [3]IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri", Milan, Italy; [4]CardioGenx, Rotterdam, Netherlands; [5]Bioneer, Horsholm, Denmark; [6]Icelandic Heart Association, Kopavogur, Iceland; [7]TNO, Zeist, Netherlands; [8]ImaBiotech, Billerica, Massachusetts; [9]AstraZeneca R&D, Gothenburg, Sweden*

WOC am 10:10 **Simultaneous detection of protein target engagement and functional readout for in-depth characterization of targeted protein degraders**; Alexey L Chernobrovkin[1]; Daniele Amadio[1]; Cindy Caceres Körner[1]; Tomas Friman[1]; Johan Lengqvist[1]; Isabel Martin Caballero[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

WOD am: Informatics: Data-Independent Acquisition

Chair: Brian Searle (Institute for Systems Biology)

WOD am 08:30 **Strategies to improve reproducibility of large-scale data-independent acquisition mass spectrometry measurements acquired on multiple instruments over an extended period**; Rebecca C Poulos[1]; Peter G Hains[1]; Rohan Shah[1]; Natasha Lucas[1]; Dylan Xavier[1]; Srikanth S Manda[1]; Asim Anees[1]; Jennifer MS Koh[1]; Sadia Mahboob[1]; Max Wittman[1]; Steven G Williams[1]; Erin K Sykes[1]; Michael Hecker[1]; Michael Dausmann[1]; Merridee A Wouters[2]; Keith Ashman[2]; Jean Yang[3]; Peter Wild[4, 5]; Anna Defazio[6, 7, 8]; Rosemary Balleine[1]; Brett Tully[1]; Ruedi Aebersold[9, 10]; Terence P Speed[11, 12]; Yansheng Liu[13, 14]; Roger R Redel[1]; Philip J Robinson[1]; Qing Zhong[1]; *[1]Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; [2]Sciex, 2 Gilda Court, Mulgrave, Australia; [3]School of Mathematics and Statistics, The University of Sydney, Sydney, Australia; [4]Dr. Senckenberg Institute of Pathology, University Hospital Frankfurt, Frankfurt am Main, Germany; [5]Department of Pathology and Molecular Pathology, University Hospital Zurich, Zurich, Switzerland; [6]Centre for Cancer Research, Westmead Institute for Medical Research, Westmead, Australia; [7]Faculty of Medicine and Health, The University of Sydney, Wesmead, Australia; [8]Department of Gynaecological Oncology, Westmead Hospital, Westmead, Australia; [9]Department of Biology, Institute of Molecular Systems Biology, ETH Zürich, Zurich, Switzerland; [10]Faculty of Science, University of Zürich, Zurich, Switzerland; [11]Bioinformatics Division, Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; [12]Department of Mathematics and Statistics, University of Melbourne, Melbourne, Australia; [13]Department of Pharmacology, Yale University School of Medicine, New Haven, CT; [14]Yale Cancer Biology Institute, Yale University, West Haven, CT*

WOD am 08:50 **Deep learning enables automated and extensible peak group identification for multi-transition chromatogram-based data-independent acquisition data analysis**; Leon L Xu[1, 2, 3]; Hannes L Röst[1, 2, 3]; *[1]University of Toronto, Toronto, ON; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON; [3]The Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

WOD am 09:10 **Multidimensional data extraction from scanning quadrupole SWATH data**; Gordana Ivosev[1]; Nic Bloomfield[1]; Stephen Tate[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, ontario*

WOD am 09:30 **Skyline integrates the Prosit prediction server for proteome-wide DIA data analysis using on-demand fragment intensity and iRT prediction**; Tobias Rohde[1]; Tobias Schmidt[2]; Nicholas Shulman[1]; Johannes Rank[3]; Bernhard Kuster[2]; Michael J MacCoss[1]; Mathias Wilhelm[2]; Brendan Maclean[1]; *[1]Univ of Washington,*

Seattle, WA; [2]*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany;* [3]*Technical University of Munich (TUM), Garching, Germany*

WOD am 09:50 **Removing the hidden data dependency of DIA with predicted spectral libraries**; Bart Van Puyvelde[1, 2]; Sander Willems[1, 2]; Ralf Gabriels[3, 4]; Simon Daled[1, 2]; Laura De Clerck[1, 2]; Sofie Vande Casteele[1, 2]; An Staes[5, 6]; Francis Impens[7]; Dieter Deforce[1, 2]; Lennart Martens[4]; Sven Degroeve[4]; Maarten Dhaenens[1, 2]; [1]*Ghent University, Faculty of Pharmaceutical Sciences, Ghent, Belgium;* [2]*ProGenTomics, Ghent, Belgium;* [3]*Ghent University, Ghent, Belgium;* [4]*VIB - UGent Center for Medical Biotechnology, Gent, Belgium;* [5]*VIB - Department of Medical Protein Research, Ghent, Belgium;* [6]*VIB - Proteomics Core, Ghent, Belgium;* [7]*VIB - Proteomics Core, Ghent, Belgium*

WOD am 10:10 **End-to-End Phenotype Prediction using Data Independent Acquisition Mass Spectrometry Tensor**; Fangfei Zhang[1]; Shaoyang Yu[2]; Lirong Wu[2]; Zelin Zang[1]; Yaoting Sun[1]; Yi Xiao[1]; Ziqing Li[1]; Zhongzhi Luan[3]; Tiannan Guo[1]; [1]*Westlake University, Hangzhou, China;* [2]*Westlake University, Hangzhou, China;* [3]*Beihang University, Beijing, China*

WOE am: GC/MS, GCxGC/MS, GC-MS/MS, and GC/HRMS

Chair: Hannah Liberatore (U.S. Environmental Protection Agency)

WOE am 08:30 **Finding Needles in a Haystack: Pesticide Analysis in Hemp with GCxGC and High Resolution Mass Spectrometry**; Todd Richards[1]; Joe Binkley[2]; Christina Kelly[2]; [1]*LECO, St. Joseph, MI;* [2]*LECO Corporation, Saint Joseph, MI*

WOE am 08:50 **Cannabinoids Analysis by GC-MS with Cold EI**; Aviv Amirav[1, 2]; Alexander B. Fialkov[3]; Tal Alon[2, 3]; Ksenia Margolin-Eren[3]; Benjamin Neumark[3]; [1]*Tel-Aviv University, Tel-Aviv, Israel;* [2]*Aviv Analytical, Hod Hasharon, Israel;* [3]*Tel Aviv University, Tel Aviv, Israel*

WOE am 09:10 **Bio-oil's isomeric compositions and their reactivity revealed by gas chromatography coupled to Fourier transform ion cyclotron resonance mass spectrometry**; Diana Catalina Palacio Lozano[1]; Hugh E. Jones[1]; Remy Gavard[1]; Mary J. Thomas[1]; Claudia X. Ramirez[2]; Christopher A. Wootton[1]; Jose Aristobulo Chaparro[3]; Peter B O'Connor[1]; Simon E. F. Spencer[1]; David Rossell[4]; Enrique Mejia Ospino[2]; Matthias Witt[5]; Mark P. Barrow[1]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*Universidad Industrial de Santander, Santander, Colombia;* [3]*Instituto Colombiano del Petroleo (ICP-Ecopetrol), Piedecuesta, Colombia, Colombia;* [4]*Universitat Pompeu Fabra, Barcelona, Spain;* [5]*Bruker, Bremen, Germany*

WOE am 09:30 **Non-targeted detection of fluorinated compounds using dielectric barrier discharge nano-electrospray ionization**; Kunyu Zheng[1]; Joseph E. Lesniewski[1]; Michael J. Dolan Jr[1]; Wanqing Li[1]; Tyler Metallo[1]; Kaveh Jorabchi[1]; [1]*Georgetown University, Washington, DC*

WOE am 09:50 **Delivering quality data in breath biomarker discovery by TD-GCxGC-TOF MS**; Laura Mcgregor[1]; Nick Bukowski[1]; Pete Grosshans[1]; Bob Green[1]; Anthony Buchanan[1]; David Bowman[2]; [1]*SepSolve Analytical, Peterborough, United Kingdom;* [2]*SepSolve Analytical, Waterloo, ON*

WOE am 10:10 **Lend Me Your Ears: Two-Dimensional Gas Chromatography-Mass Spectrometric Analysis of Earwax for Disease Diagnosis**; Rabi A Musah[1]; Allix M. Coon[1]; John Dane[2]; Robert B Cody[2]; [1]*University at Albany - SUNY, Albany, NY;* [2]*JEOL USA, Inc., Peabody, MA*

WOF am: Top Down Protein Analysis

Chair: Laura Herring (UNC-Chapel Hill)

WOF am 08:30 **A Quantitative Atlas of the Histone Proteoforms of the Brain and Applications to Disease**; Tao Wang[1]; Matthew V. Holt[1]; Nikit Venishetty[2]; Nicolas L. Young[1]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Rice University, Houston, TX*

WOF am 08:50 **Characterizing Large Heart Proteoforms (Up to 223 kDa) by Novel Top-down Proteomic Strategy**; Trisha Tucholski[1]; Kyle A. Brown[1]; Jake A. Melby[1]; Ying Ge[1]; [1]*University of Wisconsin-Madison, Madison, WI*

WOF am 09:10 **FLASHDeconv: ultrafast high-quality deconvolution for top-down MS1/MS2 spectra**; Kyowon Jeong[1]; Maša Babović[2]; Jihyung Kim[1]; Pavel V Shliaha[2]; Sebastian Gibb[3]; Ole N Jensen[2]; Oliver Kohlbacher[1, 4, 5]; [1]*University of Tübingen, Tübingen, Germany;* [2]*University of Southern Denmark, Odense, Denmark;* [3]*University Medicine Greifswald, Greifswald, Germany;* [4]*Max Planck Institute for Developmental Biology, Tübingen, Germany;* [5]*University Hospital Tübingen, Tübingen, Germany*

WOF am 09:30 **Application of cylindrical FAIMS for top-down identification of proteins directly from bacterial colonies by LESA MS**; Jana Havlikova[1]; Robin C. May[1]; Iain B. Styles[1]; Helen J. Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

WOF am 09:50   **Predicting electrophoretic mobility of proteoforms for large-scale top-down proteomics**; Daoyang Chen[1]; Rachele Lubeckyj[1]; Zhichang Yang[1]; Elijah Mccool[1]; Xiaojing Shen[1]; Qianjie Wang[1]; Tian Xu[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

WOF am 10:10   **Denatured/Native Capillary Electrophoresis and Top-Down Proteomics for In-depth Proteoform Characterization**; Kevin Jooss[1]; Rafael D Melani[1]; Luis F Schachner[1]; Nicholas W Bateman[2]; Thomas P Conrads[2, 3]; Paul M Thomas[1]; Philip D Compton[1]; Neil L Kelleher[1]; [1]*Northwestern University, Evanston, IL/60208;* [2]*Women's Health Integrated Research Center at Inova Health System, Annandale, VA/22003;* [3]*Women's Service Line, Inova Health System, Falls Church, VA/22042*

WOG am: Food Safety & Chemistry: Innovations

Chair: Tarun Anumol (Agilent Technologies)

WOG am 08:30   **More than QuEChERS is the QuEChERSER Mega-Method for Analysis of Pesticides, Veterinary Drugs, and Other Contaminants in Foods**; Steven J Lehotay; *USDA ARS, Wyndmoor, PA*

WOG am 08:50   **Significant improvements to the LC/MRM-based detection of herbicides using iTrEnDi**; Christian A Rosales[1]; Samuel W Shields[2]; Chelsey Aulenback[1]; Krysten Sheedy[1]; Karl V Wasslen[1]; Erdim Sertoglu[3]; Kym Faull[3]; Jeffrey M Manthorpe[1]; Jeffrey C Smith[1]; [1]*Carleton University, Ottawa, ON;* [2]*University of Texas Austin, Austin, TX;* [3]*University of California, Los Angeles, Los Angeles, CA*

WOG am 09:10   **A 3D Mass Spectrometry-based Method for the de Novo Structural Elucidation of Polysaccharides**; Juan J Castillo[1]; Ace G. Galermo[2]; Matthew J. Amicucci[2]; Eshani Nantida[2]; Ye Chen[1]; Carlito B Lebrilla[2]; [1]*University of California, Davis, Davis, CA;* [2]*University of California Davis, Davis*

WOG am 09:30   **Development of a standard quality control mixture for evaluating non-targeted liquid chromatography/high resolution mass spectrometry (LC/HR-MS) method performance**; Christine Fisher[1]; Jacob H. Premo[1]; Ann M. Knolhoff[1]; [1]*FDA, College Park, MD*

WOG am 09:50   **Evaluation of the segmented non-target data acquisition (SWATH/vDIA) in QToF and QOrbitrap for pesticide residue analysis**; Lukasz Rajski[1]; Iciar Beraza[1]; María José Gómez Ramos[1]; Amadeo R. Fernández-Alba[1]; [1]*European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables. University of Almeria, Agrifood Campus of International Excellence (ceiA3), Almeria, Spain*

WOG am 10:10   **Determination of Decomposition in Seafood Products by High-Resolution Mass Spectrometry with Sensory-Driven Modeling**; Randy Self[1]; Michael G. McLendon[1]; Christopher M. Lock[1]; [1]*U.S. FDA, Bothell, WA*

WOH am: Energy, Petroleum, and Biofuels: Instrumentation and Applications

Chair: Diana Palacio Lozano (University of Warwick)

WOH am 08:30   **Revisiting the Yen-Mullins Model of Petroleum Asphaltenes**; Ryan P Rodgers[1, 2]; Martha L Chacón-Patiño[1]; Sydney F Niles[2]; Alan G Marshall[1, 2]; [1]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [2]*Florida State University, Tallahassee, FL*

WOH am 08:50   **Novel four dimensional approach for the structural characterization of neutral nitrogen compounds using UHPLC-IM-QqTOF analysis on pre-fractionated vacuum gas oils**; Julie Guillemant[1]; Alexandra Berlioz-Barbier[1]; Marion Lacoue-Nègre[1]; Luis Pereira De Oliveira[1]; Jean-François Joly[1]; Ludovic Duponchel[2]; [1]*IFP Energies Nouvelles, Solaize, France;* [2]*Univ. Lille, CNRS, UMR 8516 - LASIR, Lille, France*

WOH am 09:10   **Comprehensive Screening of polycyclic aromatic hydrocarbon like compounds using GC-APLI-TIMS-TOF MS/GC-EI-MS**; Clement Ajibade Olanrewaju[1]; Cesar E Ramirez[2]; Francisco A. Fernandez-Lima[1]; [1]*Florida International University, Miami, FL;* [2]*Advance Mass Spectrometry Facility, Florida International University,, Miami, FL 33199.*

WOH am 09:30   **GC-SICRIT-HRMS for detailed analysis of saturated and unsaturated components in complex hydrocarbon mixtures**; Markus Weber[1]; Jan-Christoph Wolf[2]; Christoph Haisch[1]; [1]*TU Munich, Munich, Germany;* [2]*Plasmion GmbH, Augsburg, Germany*

WOH am 09:50   **Biomass Comparison, Characterization, and Quantification with Analytical Pyrolysis GCxGC-MS**; Brittany D.M. Hodges[1]; Amber N. Hoover[1]; Chenlin Li[1]; Gary S. Groenewold[1]; Christopher A. Zarzana[1]; Lynn M. Wendt[1]; Kyle Rigg[1]; Allison E. Ray[1]; [1]*Idaho National Laboratory, Idaho Falls, ID*

WOH am 10:10   **High Resolution Orbitrap Mass Spectrometry Analysis of Oxygenated Hydrocarbons Found in Fresh Water Contaminated by a Crude Oil Spill**; Nicole E. Heshka[1]; Kerry M. Peru[2]; John V. Headley[2]; Heather D. Dettman[1]; [1]*Natural Resources Canada, CanmetENERGY, Devon, AB;* [2]*Environment and Climate Change Canada, Saskatoon, SK*

WOA pm: Native MS in Structural Biology

Chair: David Schriemer (University of Calgary)

WOA pm 02:30 **The Structures and Stabilities of Cytochrome P450 – Drug Complexes Depend upon Their Local Lipid Environments**; Kristine F. Parson[1]; Katherine Gentry[2]; Carlo Barnaba[2]; Marina Sarcinella[1]; Colleen M. Riordan[1]; Sugyan Dixit[1, 3]; Sarah M Fantin[1]; Varun V. Gadkari[1]; Ayyalusamy Ramamoorthy[2]; Ryan C. Bailey[1]; Brandon T Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan; [2]Biophysics Program and Department of Chemistry at University of Michigan, Ann Arbor, MI; [3]Department of Pharmacology, Feinberg School of Medicine, Northwestern University,, Chicago, Illinois*

WOA pm 02:50 **Native Mass Spectrometry and Surface Induced Dissociation Complement Cryo-Electron Microscopy for Structural Elucidation of a Heterogeneous Pseudo-enzyme Complex**; Mowei Zhou[1]; Chen Du[2]; Zachary Vanaernum[2]; Irina Novikova[1]; Aivett Bilbao[1]; Vicki H. Wysocki[2]; Hanjo Hellmann[3]; James Evans[1, 3]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]The Ohio State University, Columbus, OH; [3]Washington State University, Pulman, WA*

WOA pm 03:10 **Protein ion conformations after electrospray ionization – a study with soft-landing and electron microscropy**; Jingjin Fan[1]; Zi Yang[2, 3]; Xiao Fan[2, 3]; Penglong Lian[1]; Hongwei Wang[2, 3]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Ministry of Education Key Laboratory of Protein Sciences, Beijing Advanced Innovation Center for Structural Biology, School of Life Sciences, Tsinghua University, Beijing, China; [3]Tsinghua-Peking Joint Center for Life Sciences, Tsinghua University, Beijing, China*

WOA pm 03:30 **An isotope depletion strategy for improved high resolution native mass spectrometry of metalloprotein complexes**; Kelly J. Gallagher[1]; Jennifer Ross[1]; C. Logan Mackay[1]; David P. A. Kilgour[2]; Jon Marles-Wright[3]; David J Clarke[1]; *[1]University of Edinburgh, Edinburgh, United Kingdom; [2]Nottingham Trent University, Nottingham, United Kingdom; [3]Newcastle University, Newcastle-upon-Tyne, United Kingdom*

WOA pm 03:50 **Lipids are very basic in the gas phase: implications for native mass spectrometry**; Jesse W Wilson[1]; Zachary M. Miller[1]; J. Diana Zhang[2]; Micah T. Donor[1]; Amber D. Rolland[1]; Samantha O. Shepherd[1]; William A. Donald[2]; James S. Prell[1]; *[1]University of Oregon, Eugene, OR; [2]University of New South Wales, Sydney, Australia*

WOA pm 04:10 **Empty Slot.** Stay tuned for promoted selection to be made.

WOB pm: Informatics: Innovations

Chair: Riccardo Spezia (Sorbonne Université & CNRS)

WOB pm 02:30 **Spectrum acquisition and evaluation for building the NIST tandem MS library 2020**; Yuxue Liang[1]; Pedatsur Neta[1]; Xiaoyu Yang[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

WOB pm 02:50 **Fast, Flexible and Feature-Rich Computation of Peptide and Proteoform Posterior Error Probabilities Using Binary Decision Trees in MetaMorpheus**; Michael R. Shortreed[1]; Lei Lu[1]; Robert J. Millikin[1]; Rachel M. Miller[1]; Leah V. Schaffer[1]; Zach Rolfs[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin, Madison, WI*

WOB pm 03:10 **Instantly scalable mass spectrometry data storage and inspection in the cloud**; Jessica Henning[1, 2]; Katie Lindner[2]; Rob Smith[2]; *[1]Prime Labs, Inc., Missoula, MT; [2]University of Montana, Missoula, MT*

WOB pm 03:30 **AUTOMATED, WEB-BASED ANALYSIS AND VISUALISATION OF TANDEM ION MOBILITY MASS SPECTROMETRY DATA**; Tristan Cragnolini[1, 2]; Charles Eldrid[2]; Hannah M. Britt[2]; Thomas Menneteau[2]; Aisha Ben-Younis[2]; Konstantinos Thalassinos[1, 2]; *[1]Birkbeck College, University of London, London, United Kingdom; [2]University College London, London, United Kingdom*

WOB pm 03:50 **Graph-based machine learning interprets and predicts diagnostic isomer-selective ion-molecule reactions in tandem mass spectrometry**; Jonathan A. Fine[1]; Judy K-Y. Liu[1]; Armen G. Beck[1]; Kawthar Z. Alzarieni[1]; Victoria M. Boulos[1]; Xin Ma[1]; Hilkka I. Kenttämaa[1]; Gaurav Chopra[1]; *[1]Purdue University, West Lafayette, IN*

WOB pm 04:10 **GlyCat: A Skyline tool featuring glycan spectral catalogs for automated analysis and curation of structure data**; Christopher Ashwood[1]; Rebekah L Gundry[1]; *[1]CardiOmics Program, Center for Heart and Vascular Research; Division of Cardiovascular Medicine; and Department of Cellular and Integrative Physiology, University of Nebraska Medical Center, Omaha, NE, 68198*

	WOC pm: Forensics: Innovations and Applications
	Chair: A Bakarr Kanu (Washington State University)

WOC pm 02:30   **Birds of a Feather: Species Identification of Endangered Macaws Using Direct Analysis in Real Time–Mass Spectrometry and Machine Learning**; Meghan G. Appley[1]; Samira Beyramysoltan[1]; Rabi A. Musah[1]; [1]*University at Albany, Albany, NY*

WOC pm 02:50   **Fieldable Assay for the Analysis of Organophosphorus Compounds in Flies for Chemical Defense Applications**; Sarah Dowling[1]; Christine Skaggs[1]; Charity Owings[1]; Charles Sexton[1]; Christine Picard[1]; Nicholas Manicke[1]; [1]*Indiana University Purdue University Indianapolis, Indianapolis, IN*

WOC pm 03:10   **Targeted Proteomics for the Detection of Genetically Variant Peptides in Human Identification**; Glendon J Parker[1]; Zachary C Goecker[1]; Kevin M Legg[2]; Michelle R R Salemi[1]; Anthony W Herren[1]; Brett S Phinney[1]; Robert H Rice[1]; Heather E Mckiernan[2]; [1]*University of California Davis, Davis;* [2]*Center for Forensic Science Research and Education, Willow Grove, PA*

WOC pm 03:30   **Determining Fingerprint Age with Mass Spectrometry Imaging via Ambient Ozonolysis of Triacylglycerols**; Paige Hinners[1]; Andrew E Paulson[1]; Young Jin Lee[1]; [1]*Iowa State University, Ames, IA*

WOC pm 03:50   **Mass spectrometry-based identification of body fluids for forensic purposes**; Katalin Barkovits[1]; Sascha Roocke[1]; Jennifer Stepien[1]; Kathy Pfeiffer[1]; Stephan Kuhlmann[2]; Annette Dorn[3]; Katrin Marcus[1]; [1]*Ruhr-University, Faculty of Medicine, Medizinisches Proteom-Center, Bochum, Germany;* [2]*Landeskriminalamt Nordrhein-Westfalen, Dez. 52.4 - Serologie, DNA-Analysen, Düsseldorf, Germany;* [3]*Bayerisches Landeskriminalamt, Abteilung II Sachgebiet 203 - Forensische DNA-Analytik, Munich, Germany*

WOC pm 04:10   **Forensic blood-spot age prediction by mass-spectrometry based proteomics**; Tom D Schneider[1]; Jonas Grossmann[2]; Bernd Roschitzki[2]; Thomas Kraemer[1]; Andrea E Steuer[1]; [1]*Zurich Institute of Forensic Medicine, University of Zurich, Zurich, Switzerland;* [2]*Functional Genomics Center, University/ETH, Zurich, Switzerland*

	WOD pm: Imaging: Pharmaceuticals, Metabolites, and Lipids
	Chair: Malcolm Clench (Sheffield Hallam University)

WOD pm 02:30   **Visualizing metabolites related to plant-pathogen interactions with high-resolution AP-SMALDI MSI**; Dhaka Bhandari[1]; Laura Righetti[2]; Sven Gottwald[1]; Chiara Dall'asta[2]; Bernhard Spengler[1]; [1]*Justus Leibig University Giessen, Giessen, Germany;* [2]*University of Parma, Parma, Italy*

WOD pm 02:50   **Interrogating Skin Cancer Pathology using Mass Spectrometry Imaging**; Kelly Dimovska Nilsson[1]; Noora Neittaanmäki[2, 3]; Marwa Munem[1]; Oscar Zaar[4, 5]; Tina B Angerer[6]; John Paoli[4, 5]; John S Fletcher[1]; [1]*Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg, Sweden;* [2]*Department of Clinical Pathology, Institute of Clinical Sciences, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden;* [3]*Region Västra Götaland, Sahlgrenska University Hospital, Department of Pathology, Gothenburg, Sweden;* [4]*Department of Dermatology and Venereology, Institute of Clinical Sciences, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden;* [5]*Region Västra Götaland, Sahlgrenska University Hospital, Department of Dermatology and Venereology, Gothenburg, Sweden;* [6]*Department of Bioengineering, University of Washington, Seattle, Washington*

WOD pm 03:10   **Co-registration of MALDI-MS and LA-ICP-MS images to better understand nanomaterial biodistributions in tissues**; Laura Castellanos-García[1]; Kristen N Sikora[1]; Richard W Vachet[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

WOD pm 03:30   **The role of Signaling Sphingolipids in the inflammatory response and granuloma formation duringMtbinfection: Potential for new host-directed therapy**; Carter Louise Carter[1]; Veronique Dartois[1]; [1]*Hackensack Meridian Health, Nutley, NJ*

WOD pm 03:50   **Implementing DESI-MS Imaging in Pharmaceutical Product Development: Methods and Challenges**; Josey Ellen Topolski[1]; Elizabeth Pierson[1]; [1]*Merck & Co., Inc., Rahway, NJ*

WOD pm 04:10   **On-tissue derivatization techniques for MALDI MS imaging of carbon-carbon double bond positional isomers of phospholipids**; Antonin Bednarik[1]; Jan Preisler[1]; Dominika Bezdekova[1]; Jiri Stajer[1]; Vadym Vadym Prysiazhnyi[1]; Michal Hendrych[2]; Jens Soltwisch[3]; Klaus Dreisewerd[3]; [1]*Department of Chemistry, Masaryk University, Brno, Czech Republic;* [2]*Masaryk University, Brno, Czech Republic;* [3]*Institute of Hygiene, University of Muenster, Muenster, Germany*

	WOE pm: Hydrogen-Deuterium Exchange MS: Innovations
	Chair: Touradj Solouki (Baylor University)

WOE pm 02:30   **HDX-MS with electrochemical reduction allows analysis of the insulin-like growth factor receptor and its interaction with blood-brain barrier crossing antibodies**; Joey Sheff[1]; Gerard Comamala[2]; Feng Ni[1]; Ping Xu[1]; Ping Wang[1]; Melanie Arbour[1]; Jennifer Hill[1]; Luke Masson[1]; Kristin Kemmerich[1]; John Kelly[1]; Kasper Rand[2]; Danica Stanimirovic[1]; [1]*National Research Council Canada, Ottawa, ON;* [2]*University of Copenhagen, Copenhagen, Denmark*

WOE pm 02:50   **Protein Dynamics, Unfolding, and Aggregation: A Thermodynamic Framework for Temperature-Dependent HDX-MS Experiments**; Nastaran N. Tajoddin[1]; Lars Konermann[1]; [1]*Univ. of Western Ontario, London, ON*

WOE pm 03:10   **Hydrogen-Deuterium exchange MS reveals the conformational dynamics of lipopolysaccharide outer membrane insertase LptDE**; Francesco Fiorentino[1]; Joshua B Sauer[1]; Xing Yu Qiu[1]; Phillip J Stansfeld[2]; Jani Reddy Bolla[1]; Carol V Robinson[1]; [1]*University of Oxford, Oxford, United Kingdom;* [2]*University of Warwick, Coventry, United Kingdom*

WOE pm 03:30   **Remodeling of the Binding Site of Nucleoside Diphosphate Kinase Revealed by X-ray Structure and HDX-MS**; Alain Dautant[1]; Julien Henri[2]; Philippe Meyer[2]; Thomas E. Wales[3]; John R. Engen[3]; Florian Georgescauld[3]; [1]*Université de Bordeaux, CNRS, Institut de Biochimie et Génétique Cellulaires, UMR5095, Bordeaux, France;* [2]*Sorbonne Universités, UPMC Univ. Paris 06, CNRS, Laboratoire de Biologie Moléculaire et Cellulaire des Eucaryotes, UMR8226, Institut de Biologie Physico-Chimique, Paris, France;* [3]*Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA*

WOE pm 03:50   **Integrated structural proteomic techniques shed light on RORγ response element recognition and ligand binding**; Tim Strutzenberg[1]; Scott J. Novick[1]; Ruben Garcia-Ordonez[1]; Mi Ra Chang[1]; Patrick R. Griffin[1]; [1]*The Scripps Research Institute, Jupiter, FL*

WOE pm 04:10   **Probing the Fragmentation Mechanisms of Deprotonated Lignin Model Compounds by Using Tandem Mass Spectrometry**; Jifa Zhang[1]; Erlu Feng[1]; Wanru Li[1]; John J Nash[1]; Hilkka I Kenttämaa[1]; [1]*Purdue University, West Lafayette*

	WOF pm: Quantitative Proteomics in Systems Biology
	Chair: Rena Robinson (Vanderbilt University)

WOF pm 02:30   **An Update on the Development of Quantitative MRM Assays for the Large-scale Measurement of Proteins from 20 Mouse Tissues**; Sarah A. Michaud[1]; Angela M. Jackson[1]; Jamie C. Mcguire[1]; Helena Pětrošová[1]; Yassene Mohammed[1, 2]; Olga Shevchuk[3]; Ingo Feldmann[3]; Albert Sickmann[3]; Christoph H. Borchers[4, 5, 6]; [1]*University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC;* [2]*Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands;* [3]*Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany;* [4]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [5]*Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC;* [6]*Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

WOF pm 02:50   **Study design considerations in the quantitative analysis of brain tissue for the analysis of Alzheimer's disease**; Gennifer Merrihew[1]; Julia Robbins[1]; Jea Park[1]; Deanna L Plubell[1]; Vagisha Sharma[1]; Thomas J. Montine[2]; Michael J MacCoss[1]; [1]*University of Washington, Seattle, WA;* [2]*Stanford University, Stanford, CA*

WOF pm 03:10   **Beyond BioPlex: Profiling Diversity across Cell-specific Protein Interaction Networks**; Laura Pontano Vaites[1]; David P Nusinow[1]; Jose Navarrete-Perrea[1]; Sipei Fu[1]; Fana Gebreab[1]; Arvene Golbazi[1]; Eila Maenpaa[1]; Keegan Stricker[1]; Alexandra Thornock[1]; Sanjukta Guha Thakurta[1]; Melanie P. Gygi[1]; Devin K Schweppe[1]; Joao A. Paulo[1]; J. Wade Harper[1]; Steve Gygi[1]; Edward L. Huttlin[1]; [1]*Harvard Medical School, Boston, MA*

WOF pm 03:30   **Quantitative Top-down MS Analysis of Serum Autoantibody Repertoire in Systemic Lupus Erythematosus (SLE)**; Zhe Wang[1]; Mulin Fang[1]; Kellye A Cupp-Sutton[1]; Xiaowen Liu[2]; Ken Smith[3]; Si Wu[1]; [1]*University of Oklahoma, Dept. of Chem & Biochem, Norman, OK;* [2]*IUPUI, Indianapolis, IN;* [3]*Oklahoma Medical Research Foundation, Oklahoma City, OK*

WOF pm 03:50   **Investigating host-pathogen interactions between Apis mellifera and Nosema ceranae using mass spectrometry-based proteomics.**; Mopelola O. Akinlaja[1, 2]; Leonard J. Foster[1, 2]; [1]*University of British Columbia, Vancouver, BC;* [2]*Michael Smith Laboratories, Vancouver, BC*

WOF pm 04:10   **The thermal proteome landscape of Escherichia coli**; Andre Mateus[1]; Johannes F. Hevler[1]; Jacob Bobonis[1]; Nils Kurzawa[1]; Malay Shah[1]; Karin Mitosch[1]; Camille V. Goemans[1]; Dominic Helm[1]; Frank Stein[1]; Athanasios Typas[1]; Mikhail M. Savitski[1]; [1]*European Molecular Biology Laboratory, Heidelberg, Germany*

WOG pm 02:30   **LC/QTOF-MS Identifies Unknowns in Wildfire Ash and Water Samples**; <u>Michael Thurman</u>[1]; Imma Ferrer[1]; Jerry Zweigenbaum[2]; Sheila F. Murphy[3]; Jackson P. Webster[4]; Fernando Rosario-Ortiz[5]; [1]*University of Colorado, Boulder, CO;* [2]*Agilent Technologies, Wilmington, DE19720;* [3]*U.S. Geological Survey, Boulder, CO;* [4]*California State College, Chico, Chico, CA;* [5]*University of Colorado - Boulder, Boulder, CO*

WOG pm 02:50   **Confirmation of Contaminants from Serum Suspect Screening Analysis**; <u>Ting Jiang</u>[1, 2]; Miaomiao Wang[1]; Aolin Wang[3]; Dimitri Abrahamsson[3]; Weixin Kuang[1, 2]; Dana Goin[3]; Rachel Morello-Frosch[3]; June-Soo Park[1]; Tracey Woodruff[3]; [1]*California DTSC, Berkeley;* [2]*Public Health Institute, Oakland, CA;* [3]*Department of Obstetrics, Gynecology and Reproductive Sciences, University of California, San Francisco, San Francisco, CA*

WOG pm 03:10   **Co-occurrence of azole antifungals and azole resistant fungi in wastewater effluents**; <u>Hailemariam Abrha Assress</u>[1]; Hlengilizwe Nyoni[1]; Bhekie B Mamba[1]; Titus AM Msagati[1]; [1]*UNIVERSITY OF SOUTH AFRICA(UNISA), JOHANNESBURG, South Africa*

WOG pm 03:30   **In situ localization of micropollutants and associated stress response in Populus nigra leaves using MALDI-FTICR-imaging and LC-MS/MS.**; <u>Claire Villette</u>; Loïc Maurer[1, 2]; Julien Delecolle[1]; Julie Zumsteg[1]; Mathieu Erhardt[3]; Dimitri Heintz[1]; [1]*Plant Imaging and Mass Spectrometry (PIMS), Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, Strasbourg, France;* [2]*Département mécanique des fluides et rhéologie, ICube Laboratoire des sciences de l'ingénieur, de l'informatique et de l'imagerie, UNISTRA/CNRS/ENGEES/INSA, STRASBOURG, France;* [3]*Institut de biologie moléculaire des plantes (IBMP, CNRS), Strasbourg, France*

WOG pm 03:50   **Comparison of Computationally Enhanced Non-Targeted Screening Tools: Isotopic Profile Deconvoluted Chromatogram (IPDC) Algorithm and HaloSeeker 1.0**, <u>Sadjad Fakouri Baygi</u>[1]; Sébastien Hutinet[2]; Ronan Cariou[2]; Sujan Fernando[1]; Philip K. Hopke[1]; Thomas M. Holsen[1]; Bernard S. Crimmins[1, 3]; [1]*Clarkson University, Potsdam, NY;* [2]*LABERCA Oniris INRAE, Nantes, France;* [3]*AEACS, LLC, New Kensington, PA*

WOG pm 04:10   **A New Way to Analyze Disinfection By-products in Drinking Water and Complex Matrices with Vacuum Assisted Sorbent Extraction(VASE) and GC-MS**; <u>Madison Kilpatrick</u>[1]; Victoria Noad[2]; Sage Dunham[2]; Susan Richardson[1]; [1]*University of South Carolina, Columbia, SC;* [2]*Entech Instruments, Simi Valley, CA*

WOH pm 02:30   **Tracking the Structural Evolution of 4-Aminobenzoic Acid in the Transition from Solution to the Gas Phase**; <u>Michael Hebert</u>[1]; David H. Russell[2]; [1]*Texas A&M University, DO NOT MAIL, TX;* [2]*Texas A&M University, College Station, TX*

WOH pm 02:50   **Isolation and characterisation of radical cation species utilising a cyclic ion mobility-enabled quadrupole time-of-flight (Q-cIM-oaToF) mass spectrometer**; <u>James Scrivens</u>[1]; Jackie Mosely[1]; Anirudh Sharma[1]; Martin Palmer[2]; Jakub Ujma[2]; Kevin Giles[2]; Michael T Bowers[3]; Kalju Kahn[3]; Edward Clayton[4]; [1]*Teesside University, Middlesbrough, United Kingdom;* [2]*Waters Corporation, Wilmslow, United Kingdom;* [3]*Department of Chemistry and Biochemistry, University of California Santa Barbara, Santa Barbara, CA, 93106-9510;* [4]*Consultant, Macclesfield, United Kingdom*

WOH pm 03:10   **Elucidating the Gas-phase Unfolding of Protein Complexes through Steered Molecular Dynamics Simulations**; <u>Chae Kyung Jeon</u>[1]; Sugyan M Dixit[2]; Chunyi Zhao[1]; Brandon T Ruotolo[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*Northwestern University, Chicago, IL*

WOH pm 03:30   **Deep learning the peptide universe from one million peptide collisional cross sections**; <u>Florian Meier</u>[1]; Niklas D Köhler[2]; Andreas-David Brunner[1]; Jean-Marc Wanka[2]; Eugenia Voytik[1]; Fabian J Theis[2, 3]; Matthias Mann[1, 4]; [1]*Max Planck Institute of Biochemistry, Planegg, Germany;* [2]*Helmholtz Zentrum München - Institute of Computational Biology, Neuherberg, Germany;* [3]*TU Munich, Munich, Germany;* [4]*Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark*

WOH pm 03:50   **How hot are your ions in differential mobility spectrometry?**; <u>Christian Ieritano</u>[1]; Joshua Featherstone[1]; Mircea Guna[2]; J. Larry Campbell[1, 2]; W. Scott Hopkins[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*SCIEX, Concord, ON*

WOH pm 04:10   **Pre-processing Ion Mobility Signals: Estimating and Correcting Mobility Shift in Ion Mobility Imaging Mass Spectrometry Experiments**; <u>Lukasz Migas</u>[1]; Emilio Rivera[2, 3]; Katerina V. Djambazova[2, 4]; Elizabeth Kathleen Neumann[2, 3]; Leonoor Ella Marie Tideman[1]; Nathan Heath Patterson[2, 3]; Richard M Caprioli[2, 3, 4, 5, 6]; Jeffrey M Spraggins[3, 4, 7]; Raf Van De Plas[1, 3, 7]; [1]*Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands;* [2]*Mass Spectrometry Research Center, Nashville, TN;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [5]*Department of Medicine, Vanderbilt University, Nashville, TN;* [6]*Department of*

Pharmacology, Vanderbilt University, Nashville, TN; [7]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN

THURSDAY AM ORALS

ThOA am: Instrumentation: Ambient Ionization and Applications

Chair: Xin Yan (Texas A&M University)

ThOA am 08:30 **Multi-functional Vacuum Ionization Source for MAI, LSI, and MALDI: Operational from AP for Comprehensive, Low-Cost Data-Mining in Mass Spectrometry**; Sarah Trimpin[1, 2]; Eric T.J. Davis[1]; Abigail Moreno-Pedraza[1]; Calvin A. Austin[1]; Kckenna J. Redding[3]; Monika Kish[4]; Ryan Sohizad[1]; Ahmed Musavi[1]; Frank S. Yenchick[1]; Marcus Simich[1]; Hussein Mokahal[1]; Mary-Kay Pflum[1]; Claudio N. Verani[1]; Trine G. Halvorsen[4]; Scott M. Grayson[3]; [1]*Wayne State University, Detroit, MI;* [2]*MSTM, LLC, Newark, Delaware;* [3]*Tulane University, New Orleans, LA;* [4]*University of Oslo, School of Pharmacy, Norway*

ThOA am 08:50 **Methods to enhance collection of out of plane ions in a cycloidal mass spectrometer**; Rafael Bento Serpa[1]; Elettra Piacentino[1]; Charles B. Parker[1]; Yuriy Zhilichev[1]; Roger P Sperline[2]; Robert Kingston[2]; Scott Tilden[2]; Justin Keogh[2]; Jeffrey T Glass[1]; Jason J Amsden[1]; M. Bonner Denton[2]; [1]*Duke University, Durham, NC;* [2]*University of Arizona, Tucson, AZ*

ThOA am 09:10 **Nanodroplets From Submicron Emitters Prevent Clustering during ESI: Evidence for the Serine Octomer in Bulk Solution**; Jacob S Jordan[1]; Evan R Williams[1, 2]; [1]*University of California, Berkeley, Berkeley, CA;* [2]*Lawrence Berkeley Laboratory, University of California, Berkeley, California*

ThOA am 09:30 **Multiplexing Electrospray Ionization Sources Using Orthogonal Injection into an Eletrodynamic Ion Funnel**; Pei Su[1]; Andrew Jearold Smith[1]; Michael Forrester Espenship[1]; Xi Chen[2]; Hugo Y. Samayoa-Oviedo[1]; Carlos Larriba-Andaluz[2]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN*

ThOA am 09:50 **Analysis of Non-Conjugated Steroids in Water using Paper Spray Mass Spectrometry**; Fred Paul Mark Jjunju[1]; Deidre Erin Damon[2, 3]; Simon Maher[3]; Abraham Badu-Tawiah[4]; [1]*University Of Liverpool, Liverpool, United Kingdom;* [2]*Department of Chemistry and Biochemistry, Ohio State University, Ohio Columbus, Ohio;* [3]*Department of Electrical Engineering & Electronics, University of Liverpool, Liverpool, United Kingdom;* [4]*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, 43210, USA, Columbus, Ohio*

ThOA am 10:10 **Fiber-based laser ablation electrospray ionization mass spectrometry for molecular profiling and metabolite gradients in anatomical regions selected by fluorescence microscopy**; Gessica Vasconcelos[1]; Sylwia Stopka[1]; Gary Stacey[2]; Akos Vertes[1]; [1]*George Washington University, Washington, DC;* [2]*University of Missouri, Columbia, MO*

ThOB am: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK

Chair: Eleanor Riches (Waters Corporation)

ThOB am 08:30 **Trapped Ion Mobility Spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) for Urine Metabolomic Profiling**; Cristina Di Poto[1]; Matthew Glover[1]; Sonja Hess[1]; Lisa H. Cazares[1]; [1]*AstraZeneca R&D, Gaithersburg, MD*

ThOB am 08:50 **Binary Modifiers for Optimized Separation and Sensitivity in Multidimensional Liquid Chromatography/Differential Mobility Spectrometry/Mass Spectrometry**; David Ruskic[1]; Gérard Hopfgartner[1]; [1]*University of Genève, Geneve, Switzerland*

ThOB am 09:10 **Shining Light on Steroidomics: UV-Catalyzed Reactions to Augment Structural Differences using Ion Mobility-Mass Spectrometry**; Samuel W Maddox[1]; Stine S.H. Olsen[1]; Christopher D. Chouinard[1]; [1]*Florida Institute of Technology, Melbourne, FL*

ThOB am 09:30 **Characterisation of pharmaceutical formulations enhanced by cyclic ion mobility separation of protomers for tandem mass spectrometry**; Jackie A Mosely[1]; James H Scrivens[1]; Anirudh Sharma[1]; Martin Palmer[2]; Jakub Ujma[2]; Kevin Giles[2]; [1]*Teesside University, Darlington, United Kingdom;* [2]*Waters Corporation, Wilmslow, United Kingdom*

ThOB am 09:50 **timsTOF Characterizations of the Esters of Disaccharides and 3-Pyridinylboronate in Positive and Negative ESI in situ**; Lei Li[1]; Pengfei Guan[1]; Pingping Wang[1]; Jun J Hu[1]; [1]*Ningbo University, Ningbo, China*

ThOB am 10:10 **Deviations from the Mason-Schamp Equation for Small Molecules; an Ion Mobility study**; Viraj Gandhi[1, 2]; Carlos Larriba Andaluz[1]; [1]*IUPUI, Indianapolis, IN;* [2]*Purdue University, West Lafayette, IN*

	ThOC am: Clinical Analysis: Innovations
	Chair: Rebekah Gundry (University of Nebraska Medical Center)

ThOC am 08:30 **In vivo Tissue Analysis in Robotic Surgery Using a Laparoscopic MasSpec Pen Device integrated to the da Vinci Surgical System**; Michael F. Keating[1]; Jialing Zhang[1]; Clara L. Feider[1]; Sascha Retailleau[2]; Robert Reid[2]; Alexander Antaris[2]; Bradley Hart[3]; Gina Tan[3]; Thomas E. Milner[1]; Kyle Miller[1]; Livia S. Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Intuitive Surgical, Sunnyvale, CA; [3]Thermo Fisher Scientific, San Jose, CA*

ThOC am 08:50 **In vivo real-time topological molecular imaging analysis by SpiderMass technology**; Nina Ogrinc[1]; Alexandre Kruszewski[2]; Paul Chaillou[2]; Philippe Saudemont[1]; Michel Salzet[1]; Christian Duriez[2]; Isabelle Fournier[1]; *[1]PRISM Inserm U1192, University of Lille, 59000 Lille, France; [2]UMR 9189 - CRIStAL - Centre de Recherche en Informatique, Signal et Automatique de Lille, University of Lille, INRIA, CNRS, Centrale Lille, Lille, France*

ThOC am 09:10 **Assessing ADME proteins in extracellular vesicles for drug therapeutics**; Xiaofeng Wu[1]; Sheri Smith[2]; Anton B Iliuk[3]; Kevin P. Bateman[2]; Joe Cannon[4]; W. Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co., Inc., West Point, PA; [3]Tymora Analytical Operations, West Lafayette, Indiana; [4]Merck & Co., West Point, PA*

ThOC am 09:30 **Development of a Paper Spray Mass Spectrometry (PS-MS) Whole Blood Extraction Cartridge**; Greta Ren[1]; Brandon Bills[1]; Nicholas Manicke[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

ThOC am 09:50 **Single-use porous polymeric thin-film device for extraction of pharmaceuticals from blood spots and other biological fluids**; Christina Bottaro[1]; Fereshteh Shahhoseini[1]; Ali Azizi[1]; Evan Langille[1]; *[1]Memorial University, St. John's, NL*

ThOC am 10:10 **A mass spectrometry-based smart-toilet for real-time health monitoring**; Benton J Anderson[1]; Ian J Miller[1]; Katherine A Overmyer[1]; Michael S Westphall[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

	ThOD am: Metabolomics: Untargeted Profiling
	Chair: Erica Forsberg (San Diego State University)

ThOD am 08:30 **Chemical cartography of the metabolic impact of chronic T. cruziinfection on cardiac tissue**; Danya A Dean[1, 2]; Gautham Gautham[2, 3]; Jair L Siqueira-Neto[4]; James H Mckerrow[4]; Pieter C. Dorrestein[4, 5, 6]; Laura-Isobel Mccall[1, 2, 7]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; [2]Laboratories of Molecular Anthropology and Microbiome Research, University of Oklahoma, Norman, OK; [3]Department of Biology, University of Oklahoma, Norman, OK; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [5]Center for Microbiome Innovation, University of San Diego, La Jolla, CA; [6]Collaborative Mass Spectrometry Innovation Center, University of San Diego, La Jolla, CA; [7]Department of Microbiology and Plant Biology, University of Oklahoma, Norman, OK*

ThOD am 08:50 **Monitoring phenyl-γ-valerolactones production following proanthocyanidins consumption to identify different human gut metabotypes**; Jacob Lessard-Lord[1]; Pier-Luc Plante[1]; Valentina Cattero[1]; Charlène Rosine Roussel[1]; Stéphanie Dudonné[1]; Yves Desjardins[1]; *[1]Centre de recherche Nutrition, Santé et Société (NUTRISS), INAF, Université Laval, Québec, Québec*

ThOD am 09:10 **Comparison of Three Common Data Acquisition Modes in Liquid Chromatography-Mass Spectrometry Based Untargeted Metabolomics**; Jian Guo[1]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC*

ThOD am 09:30 **Combination of UHPLC-MS/MS-molecular networking approach and FTICR-MS for the dereplication of Saccharomyces cerevisiae**; Olivier Perruchon[1]; Isabelle Schmitz-Afonso[1]; Cécile Grondin[2]; Serge Casaregola[2]; Carlos Afonso[1]; Abdelhakim Elomri[1]; *[1]University of Rouen-Normandy, Mont-Saint-Aignan, France; [2]Micalis Institute, INRA, CIRM-Levures, Université Paris-Saclay, Jouy-en-Josas, France*

ThOD am 09:50 **High Resolution LC-MS Analysis of Wine Samples for the Characterization of Flavonoids**; Brandon Bills[1]; Seema Sharma[1]; Ralf Tautenhahn[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThOD am 10:10 **A library of 400 metabolites for Mapping Metabolome-wide Changes in Cyanobacteria**; Damini Jaiswal[1]; Rochit Sinha[1, 2]; Pramod P Wangikar[3]; *[1]IIT Bombay, Mumbai, India; [2]BITS Pilani, Goa, Goa, India; [3]Indian Institute of Technology Bombay, Mumbai, India*

	ThOE am: MS in the Process Development Lab
	Chair: Benben Song (Pall Biotech)

ThOE am 08:30 **End-to-end automation of multi-attribute method (MAM) platform for process development and characterization of antibodies**; Yvonne Ehwang Song[1]; Stephen D'eri[1]; Martin Hoffmann[2]; Herve Dubois[3]; Anja Pfenninger[2]; Jan Wiesner[2]; Udo Roth[2]; Yann Fromentin[3]; Bradley Whittaker[1]; Marina Hincapie[1]; Annette Pieper[2]; Laurent Duhau[3]; *[1]Sanofi, Framingham, MA; [2]Sanofi, Frankfurt am Main, Germany; [3]Sanofi, Vitry Sur Seine, France*

ThOE am 08:50 **Automated feedback control of protein characteristics in a perfusion bioprocess**; James Graham[1]; John Schmitt[2]; Julia Oddo[2]; Sylwia Jozwiak[1]; Wilfred Tang[3]; Marshall Bern[3]; Eric Carlson[3]; Brandon Downey[2]; *[1]Lonza, Slough, United Kingdom; [2]Lonza LPB R&D, Bend, Oregon; [3]Protein Metrics Inc., Cupertino, CA*

ThOE am 09:10 **High-Throughput, Multi-Attribute Continuous Product Characterisation Platform for Increased Process Control Monitoring**; Noemi Dorival-Garcia[1]; Patrick Floris[1]; Jonathan Bones[1]; *[1]NIBRT, Dublin, Ireland*

ThOE am 09:30 **Point-of-need miniaturized ESI-MS for monitor and control of a bioreactor**; Richard W. Moseley[1]; Max Wong[1]; Alexander I. Mcintosh[1]; *[1]Microsaic Systems, Woking, United Kingdom*

ThOE am 09:50 **Quantitative LC-MS/MS workflow for targeted analysis of cell culture media**; Hari Kosanam[1]; Jared Kress[1]; Sha Ha[1]; Zuzana Demianova[2]; Baljit Ubhi[3]; Lei Xiong[3]; *[1]Merck, WestPoint, PA; [2]Sciex, Brea, CA; [3]SCIEX, Redwood Shores, CA*

ThOE am 10:10 **Identification of critical chemical modifications and paratope mapping by size exclusion chromatography (SEC) of stressed antibody-target complexes**; Pavel V. Bondarenko[1]; Gang Xiao[1]; Rachel Liuqing Shi[1]; Andrew Nichols[1]; Thomas M Dillon[1]; Pik Becky Chan[1]; Margaret S Ricci[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

	ThOF am: Single Cell MS
	Chairs: Ying Zhu (Pacific Northwest National Laboratory)

ThOF am 08:30 **Quantitative Measure of Amiodarone and Associated Metabolites in Single HepG2 Liver Cells Using Single Cell Printing-Liquid Vortex Capture-Mass Spectrometry**; John F. Cahill[1]; Vilmos Kertesz[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

ThOF am 08:50 **Single-Cell Mass Spectrometry Reveals Cell-to-Cell Communication in Xenopus laevis (Frog) Embryos**; Erika Portero[1]; Leena Pade[1]; Peter Nemes[1]; *[1]University of Maryland, College Park, Maryland*

ThOF am 09:10 **Single cell mass spectrometry metabolomics studies of cell heterogeneity in the infection of Chagas disease**; Yunpeng Lan[1]; Tra Nguyen[1]; Renmeng Liu[1]; Shelley S. Kane[1]; Laura-Isobel Mccall[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

ThOF am 09:30 **Combined Single Neuron Patch-Clamp/Mass Spectrometry Analyses**; Jolene Diedrich[1]; Matt Albertolle[1]; Nima Dolatabadi[1]; Swagata Ghatak[1]; Maria Talantova[1]; Stuart A Lipton[1]; John Robert Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA*

ThOF am 09:50 **Leveraging trapped ion mobility spectrometry and PASEF for single cell proteomics**; Andreas-David Brunner[1]; Florian Meier[1]; Fabian Coscia[1, 2]; Craig Whitehouse[3]; Markus Lubeck[4]; Nagarjuna Nagaraj[4]; Ole Bjeld Horning[5]; Oliver Raether[4]; Andreas Mund[2]; Nicolai Bache[5]; Melvin A. Park[3]; Matthias Mann[1, 2]; *[1]Max Planck Institute of Biochemistry, Planegg, Germany; [2]NNF Center for Protein Research, Copenhagen, Denmark; [3]Bruker Scientific LLC, Billerica, MA; [4]Bruker, Bremen, Germany; [5]Evosep Biosystems, Odense, Denmark*

ThOF am 10:10 **Improvements in sensitivity of nanoLC-MS-based deep proteomics profiling using monolithic capillary columns and the FAIMS Pro interface**; Michal Gregus[1]; Susan E. Abbatiello[1]; James Kostas[1]; Somak Ray[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

ThOG am 08:30 **Effect of Nonionic Saccharide Detergents and Supercharging Agents on Native Mass Spectrometry of Membrane Proteins**; Wonhyeuk Jung[1]; Wenzhe Chen[1]; Muhammad A. Zenaidee[1]; Pascal Egea[1]; Mark Arbing[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; [1]*UCLA, Los Angeles, CA*

ThOG am 08:50 **Uncovering the Molecular Details of G Protein-Coupled Receptor Activation**; Corinne A Lutomski[1]; Tom N Durrant[1]; Carol V Robinson[1]; [1]*University of Oxford, Oxford, United Kingdom*

ThOG am 09:10 **Mechanism of adrenergic CaV1.2 stimulation revealed by proximity proteomics**; Marian Kalocsay[1]; Guoxia Liu[2]; Steven O. Marx[2]; Steve Gygi[1]; [1]*Harvard Medical School, Boston, MA;* [2]*Columbia University College of Physicians and Surgeons, New York, NY*

ThOG am 09:30 **Top-down high-resolution mass spectrometry of larger membrane proteins: precise subunit mass analysis under conditions that eliminate non-covalent interactions**; Julian Whitelegge; *University of California LA, Los Angeles, CA*

ThOG am 09:50 **Release of membrane proteins from detergent micelles using an in-source declustering ion guide**; Kleitos Sokratous[1]; Jakub Ujma[2]; Kevin Giles[2]; Dale A. Cooper-Shepherd[2]; Idlir Liko[1]; Joseph Gault[3]; Jonathan T.S. Hopper[1]; Carol V. Robinson[3]; [1]*OMass Therapeutics LTD, Oxford, United Kingdom;* [2]*Waters Corporation, MS Research, Wilmslow, United Kingdom;* [3]*University of Oxford, Oxford, United Kingdom*

ThOG am 10:10 **Empty Slot.** Stay tuned for promoted selection to be made.

ThOH am 08:30 **Two-Dimensional Mass Spectrometry, an update**; Anisha Haris[1]; Yuko Lam[1]; Meng Li[1]; Tomos E. Morgan[1]; Bryan P. Marzullo[1]; Alina Thiesen[1]; Christopher A. Wootton[2]; Peter B. O'connor[3]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*Verdel Instruments Ltd, Coventry, United Kingdom;* [3]*University of Warwick, Coventry, United Kingdom*

ThOH am 08:50 **A Comparison of Intelligent Data-Acquisition Methods for Exposomics and Lipidomics Applications**; Jeremy Koelmel[1]; Georgia Charkoftaki[1]; Sara Nason[2]; Elizabeth Lin[1]; Vasilis Vasiliou[1]; John A. Bowden[3, 4]; Juan Aristizabal[3]; Paul Stelben[1]; Matthew Paige[1]; Krystal G. Pollitt[1]; Timothy J Garrett[5, 5]; [1]*School of Public Health, Yale University, New Haven, CT;* [2]*Departments of Environmental Sciences and Analytical Chemistry, The Connecticut Agricultural Experiment Station, New Haven, CT;* [3]*Center for Environmental and Human Toxicology & Department of Physiological Sciences, University of Florida, Gainesville, FL;* [4]*Department of Chemistry, University of Florida, Gainesville, FL;* [5]*Department of Pathology, Immunology and Laboratory Medicine, University of Florida, Gainesville, FL*

ThOH am 09:10 **An ultra-high-resolution IonStar proteomics strategy enables accurate and reproducible large-cohort quantification and outperforms the state-of-the-art SWATH-MS**; Xue Wang[1]; Liang Jin[1]; Chenqi Hu[1]; Shichen Shen[2]; Shuo Qian[2]; Yu Tian[1]; Jun Qu[2]; [1]*AbbVie, Worcester, MA;* [2]*University at Buffalo, Buffalo, NY*

ThOH am 09:30 **Opportunities and challenges for improving quantitative accuracy and precision in SILAC with DIA-MS**; Lindsay K Pino[1]; Josue Baeza[1]; Richard Lauman[1]; Benjamin A. Garcia[1]; [1]*Department of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA*

ThOH am 09:50 **High-field asymmetric waveform ion mobility spectrometry improves the depth and throughput of single-cell proteomics**; Jongmin Woo[1]; Geremy Clair[1]; Chia-Feng Tsai[1]; Sarah M. Williams[1]; Ronald J. Moore[1]; William B. Chrisler[1]; Tao Liu[1]; Richard D. Smith[1]; Ryan T. Kelly[2]; Ljiljana Pasa-Tolic[1]; Charles K Ansong[1]; Ying Zhu[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Brigham Young University, Provo, UT*

ThOH am 10:10 **Lessons Learned the Hard Way: Acquiring and Analyzing Data Independent Acquisition Proteomics Data Collected on Quadrupole-Orbitrap Mass Spectrometers**; Brian C. Searle[1]; Lindsay K Pino[2]; Seth C Just[3]; Michael J MacCoss[4]; [1]*Institute for Systems Biology, Seattle, WA;* [2]*University of Pennsylvania School of Medicine, Philadelphia, PA;* [3]*Proteome Software, Portland, OR;* [4]*University of Washington School of Medicine, Seattle, Washington*

THURSDAY PM ORALS

ThOA pm: Pharmaceuticals: Impurity Analysis	
Chair: Miryam Kadkhodayan (Geltor)	

ThOA pm 02:30 **Contribution of FAIMS and DIA for monitoring and accurately quantifying trace-level host cell protein impurities in therapeutic proteins**; Nicolas Pythoud[1]; Joanna Bons[1]; Sega Ndiaye[2]; Tabiwang Arrey[3]; Claire Dauly[2]; Alain Beck[4]; Sarah Cianférani[1]; Christine Carapito[1]; [1]*University of Strasbourg, CNRS, IPHC UMR 7178, STRASBOURG, France;* [2]*Thermo Fisher Scientific, Courtaboeuf, France;* [3]*Thermo Fisher Scientific, Bremen, Germany;* [4]*IRPF - Centre d'Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France*

ThOA pm 02:50 **Characterization and Quality Control of Synthetic Oligonucleotide Therapeutics by Mass Spectrometry: the Current and the Future**; Kui Yang[1]; Sarah Rogstad[2]; Jason Rodriguez[1]; David Keire[1]; [1]*FDA, St. Louis, MO;* [2]*FDA, College Park, MD*

ThOA pm 03:10 **Accelerated Screening for the Protection and Efficacy of Cell Treatments (ASPECT) via MALDI MS.**; Stephen C Zambrzycki[1]; Gilad Doron[2]; Monica Tran[1]; Carter K Asef[1]; Johnna Temenoff[2]; Facundo M. Fernandez[1]; [1]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA;* [2]*Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, GA*

ThOA pm 03:30 **Study of Ranitidine Stability: Quantification of N-Nitrosodimethylamine (NDMA), a Probable Carcinogen in Ranitidine Drug Products and Biological Matrices by UHPLC-MS/MS**; Eshani Nandita[1]; Ali Najafi[2]; Neelanjan Bose[2]; [1]*EMERY PHARMA, Alameda, CA;* [2]*Emery Pharma, Alameda, CA*

ThOA pm 03:50 **A novel data processing strategy for detection of low-abundance HCPs: Increased sensitivity and accuracy with fewer false-positive identifications**; Maurizio Bronzetti[1]; Jonathan Jones[2]; Peter Haberl[3]; Catherine Evans[4]; Stefano Gotta[4]; [1]*Genedata Inc, San Francisco, CA;* [2]*Genedata Ltd, Cambridge, United Kingdom;* [3]*Genedata GmbH, Munich, Germany;* [4]*Genedata AG, Basel, Switzerland*

ThOA pm 04:10 **Rapid Quantitative Analysis of Genotoxic Impurity Nitrosamines in Pharmaceuticals by Liquid Chromatography High Resolution Mass Spectrometry**; Kate Comstock[1]; Christine Skaggs[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Indiana University Purdue University Indianapolis, Indianapolis, IN*

ThOB pm: Ion Mobility: New Developments & Applications	
Chair: Ian Webb (IUPUI)	

ThOB pm 02:30 **Surface-induced Dissociation of Trapped Ion Mobility-Selected Protein Complexes**; Erin M. Panczyk[1]; Dalton T. Snyder[1]; Arpad Somogyi[1]; Mark E. Ridgeway[2]; Melvin A. Park[2]; Vicki H. Wysocki[1]; [1]*The Ohio State University, Columbus, OH;* [2]*Bruker Daltonics, Billerica, MA*

ThOB pm 02:50 **Millisecond Chiral Separation by Multidimensional IM-MS Provides Molecular and Structural Basis for Next-generation Therapy of Alzheimer's Disease**; Gongyu Li[1]; Min Ma[1]; Chae Kyung Jeon[2]; Brandon T Ruotolo[2]; Lingjun Li[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin;* [2]*University of Michigan, Ann Arbor, MI*

ThOB pm 03:10 **Fourier Transform Ion Mobility Linear Ion Trap Mass Spectrometer with Frequency Encoding to Recognize Related Compounds in a Single Acquisition**; Robert Schrader[1]; Brett M. Marsh[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN*

ThOB pm 03:30 **Some illustrations of the advances brought by high-resolution ion mobility coupled to multi-function MS capabilities in structural glycosciences**; David Ropartz[1, 2]; Mathieu Fanuel[1, 2]; Jakub Ujma[3]; Martin Palmer[3]; Kevin Giles[3]; Hélène Rogniaux[1, 2]; [1]*INRAE, UR BIA, Nantes, France;* [2]*INRAE, BIBS facility, Nantes, France;* [3]*Waters Corporation, MS Research, Wilmslow, United Kingdom*

ThOB pm 03:50 **Fourier Transform-Ion Mobility-Orbitrap Mass Spectrometry of Carbohydrates: More Signal, More of the Time**; Kristin R Mckenna[1]; Ramanarayanan Krishnamurthy[2, 3]; Charles L. Liotta[1, 2]; Brian H Clowers[4]; Facundo M. Fernandez[1, 2]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*Center for Chemical Evolution, Atlanta, GA;* [3]*The Scripps Research Institute, La Jolla, CA;* [4]*Washington State University, Pullman, WA*

ThOB pm 04:10 **Empty Slot.** Stay tuned for promoted selection to be made.

ThOC pm 02:30 **Assessment and Optimization of Denaturing and Native Microfluidic CE-MS Methods to Characterize Bispecific Antibodies**; Laura Herring[1]; Natalie K Barker[1]; Joshua Beri[1]; J. Scott Mellors[2]; St John Skilton[3]; Tracy Kuhlman[4]; Tim Jacobs[4]; [1]*UNC-Chapel Hill, Chapel Hill, NC;* [2]*908 Devices, Inc., Carrboro, NC;* [3]*Protein Metrics Inc, Cupertino, CA;* [4]*Dualogics, LLC, Durham, NC*

ThOC pm 02:50 **Rapid Characterization of Therapeutic Antibody Charge Variants Using Microchip-Based Imaged cIEF Integrated with High Resolution Mass Spectrometry**; Daniel Donnelly[1]; Bhumit Patel[1]; Douglas Richardson[1]; Mariam S Elnaggar[2]; Christopher Herring[2]; Scott Mack[2]; Erik Gentalen[2]; [1]*Merck & Co., Inc., Analytical Research and Development, Kenilworth, NJ;* [2]*Intabio, Inc., Newark, CA*

ThOC pm 03:10 **Human leukocyte antigen II immunopeptidomics in dendritic cells in response to immune-complexes of TNF with anti-TNF biotherapeutics**; Andrea Casasola-LaMacchia[1]; Robert J Seward[1]; Maria Stella Ritorto[1]; Gabrielle Bergeron[1]; Zhaojiang Lu[1]; Michael Agostino[1]; Andrew Ciarla[1]; Nathalie Ahyi-Amendah[1]; Matthew Willetts[2]; Shourjo Ghose[2]; Hai-Young Kim[1]; Tim Hickling[1]; Hendrik Neubert[1]; [1]*Pfizer Inc., Andover, MA;* [2]*Bruker Daltonics, Billerica, MA*

ThOC pm 03:30 **Development of a SWATH-Mass Spectrometry-based Proteomic Method for the Characterization of CAR-T Cell Therapy**; Camille Lombard-Banek[1, 2]; Edward J Kwee[3]; Sumona Sarkar[3]; John T Elliott[3]; John E Schiel[1, 2]; [1]*National Institute of Standards and Technology, Rockville, MD;* [2]*Institute for Bioscience and Biotechnology Research, Rockville, Maryland;* [3]*National Institute of Standards and Technology, Gaithersburg, Maryland*

ThOC pm 03:50 **Discovery and characterization of a mAb with C-terminal Fc-extension and O-glycosylation**; Harsha Gunawardena[1]; Eric Beil[1]; Andrew D Mahan[1]; Elsa Gorre[1]; Bo Zhai[1]; Hirsh Nanda[1]; [1]*JOHNSON AND JOHNSON, Spring House, PA*

ThOC pm 04:10 **Analytical characterisation of cell line and sequence differences on final product properties of biotherapeutics**; Lewis Elliott Wharram[1]; Vicky Smith[1]; Michael Anyadiegwu[1]; Jodie Clemmit[1]; John Liddell[1]; [1]*CPI, Darlington, United Kingdom*

ThOD pm 02:30 **Using Complete Hydrogen-Deuterium Exchange to Identify Unknown Compounds in Untargeted HILIC Metabolomics of Mouse Mammary Tumors**; Clayton Bloszies[1]; Brian C Defelice[2]; Megan R Showalter[3]; Tong Shen[4]; Michael R Sa[5]; Kacey Vandervorst[6]; Anastasia L Berg[6]; Kermit L Carraway III[6]; Tomas Cajka[7]; Tobias Kind[4]; Dinesh K. Barupal[4]; Oliver Fiehn[4]; [1]*UC Davis, Davis, CA;* [2]*Chan Zuckerberg Biohub, San Francisco, CA;* [3]*Metabolon, Morrisville, NC;* [4]*West Coast Metabolomics Center, UC Davis, Davis, CA;* [5]*California Northstate University, College of Medicine, Elk Grove, CA;* [6]*Department of Biochemistry and Molecular Medicine, UC Davis, Sacramento, CA;* [7]*Department of Metabolomics and Translational Metabolism, Institute of Physiology CAS, Prague, Czech Republic*

ThOD pm 02:50 **Combining Credentialing, Ion Mobility Spectrometry, and Tandem Mass Spectrometry (IMS-MS/MS) to Detect, Identify and Validate Metabolites in Untargeted Analyses**; James N. Dodds[1]; Lingjue Wang[2]; Gary Patti[2]; Erin S. Baker[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*Washington University, St. Louis, St. Louis, MO*

ThOD pm 03:10 **Application of predicted collisional cross section to metabolome databases to probabilistically describe the current and future ion mobility mass spectrometry**; Corey D Broeckling[1]; Linxing Yao[1]; Amy Sheflin[1]; Johannes P.C. Vissers[2]; Giorgis Issac[3]; Jeff Goshawk[2]; Suraj Dhungana[3]; Robert Plumb[3]; [1]*Colorado State University, Fort Collins, CO;* [2]*Waters Corporation, Wilmslow, United Kingdom;* [3]*Waters Corporation, Milford, MA*

ThOD pm 03:30 **Profiling of small polar metabolites in genetically modified Arabidopsis thaliana samples by capillary ion chromatography HR-MS**; Hannah Schöttler[1]; Heiko Hayen[1]; [1]*University of Muenster - Institute of Inorganic and Analytical Chemistry, Münster, Germany*

ThOD pm 03:50 **MxP® Quant 500 Kit with Waters Xevo® TQ-XS Mass Spectrometry for Standardized and Comprehensive Targeted Metabolomics and Lipidomics**; Ulf Sommer[1]; Hai Pham-Tuan[1]; Xenia Enkelmann[1]; Doreen Kirchberg[1]; Martin Buratti[1]; Andrew J. Peck[2]; Therese Koal[1]; [1]*BIOCRATES Life Sciences AG, Innsbruck, Austria;* [2]*Waters Corporation, Milford, Massachusetts*

ThOD pm 04:10 **Empty Slot.** Stay tuned for promoted selection to be made.

	ThOE pm: Protein-Ligand Interactions
	Chair: Tracie Williams (Centers for Disease Control and Prevention)

ThOE pm 02:30 **Unraveling the Three-dimensional Molecular Recognition Codes of Experimental and Diagnostic Antibodies by nanoESI Ion Mobility Mass Spectrometry**; Bright D. Danquah[1]; Claudia Röwer[1]; Kwabena F.M. Opuni[2]; Reham A. El-Kased[3]; Cornelia Koy[1]; Michael O. Glocker[1]; [1]*Proteome Center Rostock, Rostock, Germany; [2]School of Pharmacy, University of Ghana, Legon, Ghana; [3]The British University in Egypt, Cairo, Egypt*

ThOE pm 02:50 **Native Top-Down Mass Spectrometry of Amyloid Proteins and Their Interaction with the Aggregation Inhibiting Compound CLR01**; Carter Lantz[1]; Muhammad A. Zenaidee[1]; Jaybree Lopez[1]; Rachel R. Ogorzalek Loo[1]; Gal Bitan[1]; Joseph A. Loo[1]; [1]*University of California, Los Angeles, Los Angeles, CA*

ThOE pm 03:10 **Assembly and regulation of the chlorhexidine specific efflux pump AceI**; Jani Reddy Bolla[1]; Anna C Howes[1]; Francesco Fiorentino[1]; Carol V Robinson[1]; [1]*University of Oxford, Oxford, United Kingdom*

ThOE pm 03:30 **Peanut allergen ejection for unambiguous characterization of immunological interactions**; John P Mcgee[1]; Rafael D Melani[1]; Valerie J Winton[1]; Derek Croote[2]; Benjamin Des Soye[1]; Michael A Swift[2]; Stephen R Quake[2]; Neil L. Kelleher[1]; Philip D Compton[1]; [1]*Northwestern University, Evanston, IL/60208; [2]Stanford University, Palo Alto, CA*

ThOE pm 03:50 **Probing Host-Microbe Interactions Through Glycomic and Glycoproteomic Methods**; Ying Sheng[1]; Yixuan (axe) Xie[1]; Qiongyu Li[1]; Carlito B Lebrilla[1]; [1]*University of California, Davis, Davis, CA*

ThOE pm 04:10 **Determining the Binding Site of Molecules on Aβ42 by DFT Calculations and Fast Photochemical Oxidation of Proteins (FPOP) Mass Spectrometry**; George Mathai[1]; Saketh Chemuru[2]; Daryl Giblin[2]; Michael L. Gross[2]; [1]*Sacred Heart College, Kochi, India; [2]Department of Chemistry, Washington University in St. Louis,, st. Louis, Missouri*

	ThOF pm: Carbohydrates
	Chair: Yehia Mechref (Texas Tech University)

ThOF pm 02:30 **EED MS2-guided -MS3 on Q Exactive-Omnitrap: a novel approach toward automated, de novo glycan sequencing**; Juan Wei[1]; Dimitris Papanastasiou[2]; Mariangela Kosmopoulou[2]; Athanasios Smyrnakis[2]; Yang Tang[1, 3]; Joseph Zaia[1]; Pengyu Hong[4]; Catherine E. Costello[1, 3]; Cheng Lin[1]; [1]*Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; [2]Fasmatech Science and Technology, Athens, Greece; [3]Department of Chemistry, Boston University, Boston, MA; [4]Department of Computer Science, Brandeis University, Waltham, MA*

ThOF pm 02:50 **Glycoproteomic and imaging MS applications of an alpha 2,3 linked sialic acid targeted bioorthogal chemical labeling probe**; Richard R Drake[1]; Colin Mcdowell[1]; Connor A West[1]; Grace Grimsley[1]; Xiaowei Lu[1]; [1]*Medical University of South Carolina, Charleston, SC*

ThOF pm 03:10 **MOBILion's SLIM-Mass Spectrometry for High Resolution and High Throughput Ion Mobility Analyses of N- and O-linked Glycoprotein Glycans**; Lance Wells[1]; Kelly L. Wormwood Moser[2]; James R. Arndt[2]; Anisha Yadav[2]; Stephen Krufka[2]; Gregory Van Aken[2]; John Daniel DeBord[2]; Gregory Webster[2]; Robert Bridger[1]; Kazuhiro Aoki[1]; Jeremy Praissman[1]; Laura Maxon[2]; Michael Tiemeyer[1]; [1]*CCRC/UGA, Athens, GA; [2]MOBILion Systems Inc., Chadds Ford, PA*

ThOF pm 03:30 **Advances in Tandem Mass Spectrometry Approaches for the Structural Characterization of Sulfated Glycosaminoglycans**; Lauren E. Pepi[1]; Zachary J. Sasiene[2]; Franklin E. Leach III[1]; Praneeth M. Mendis[2]; Dustin R. Klein[3]; Pradeep Chopra[4]; Fuming Zhang[5]; Robert J. Linhardt[5]; Geert-Jan Boons[4]; Jennifer S. Brodbelt[6]; Glen P. Jackson[2]; I. Jonathan Amster[1]; [1]*University of Georgia, Athens, GA; [2]West Virginia University, Morgantown, WV; [3]Vanderbilt University, Nashville, TN; [4]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [5]Rensselaer Polytechnic Institute, Troy, NY; [6]University of Texas at Austin, Austin, TX*

ThOF pm 03:50 **Differentiating Fragmentation Pathways of Sialylated Human Milk Oligosaccharides as Magnesium Adducts by Electron Transfer/Ion Mobility/Vibrational Activation**; Anna J Diepenbrock[1]; Eric D Dodds[2]; [1]*University of Nebraska - Lincoln, Lincoln, NE; [2]University of Nebraska-Lincoln, Lincoln, NE*

ThOF pm 04:10 **Resolving positional and compositional isomers of protonated disaccharides by tandem mass spectrometry, ion mobility, and gas-phase hydrogen deuterium exchange**; Abhigya Mookherjee[1]; Sanjit (sunny) Uppal[2]; Miklos Guttman[2]; [1]*University of Washington, Seattle; [2]University of Washingtion, Seattle, Seattle, WA*

ThOG pm: Synthetic Polymers

Chair: Kevin Endres (E. I. du Pont de Nemours and Company)

ThOG pm 02:30 **Differences in MALDI ionization of neat linear and cyclic poly(L-lactide)s**; Steffen M Weidner[1]; Hans R. Kricheldorf[2]; [1]*Federal Institute for Materials Research & Testing, Berlin, Germany; [2]Universität Hamburg, Hamburg, Germany*

ThOG pm 02:50 **Comprehensive characterization of poly(lactide-co-glycolide)s combining chromatography with matrix- and surface-assisted laser desorption ionization low- and high-resolution mass spectrometry**; Thierry Nicolas Jean Fouquet[1]; Takayuki Ohmura[2]; Masataka Kotani[2]; Yasuhide Naito[3]; Delphine Crozet[4]; Pierre Giusti[4, 5]; Laurence Charles[6]; [1]*National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [2]Hamamatsu Photonics K.K., Iwata, Japan; [3]The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan; [4]Total Refining and Chemicals, Harfleur, France; [5]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; [6]Aix-Marseille Université - Institut de Chimie Radicalaire, Marseille, France*

ThOG pm 03:10 **Rethinking the Structure and Reactivity of Silicone MQ Resins**; Richard Cooper[1]; Tianlan Zhang[2]; Steven Arturo[1]; [1]*Dow, Collegeville, PA; [2]Glaukos Corporation, San Clemente, California*

ThOG pm 03:30 **Regio and stereospecific chemical depolymerization of high molecular mass polybutadiene and polyisoprene for the analysis by high resolution mass spectrometry**; Ziad Mahmoud[1]; Fabrice Bray[1]; Marie Hubert-Roux[2]; Michel Sablier[3]; Carlos Afonso[2]; Christian Rolando[1]; [1]*Université de Lille, Faculté des Sciences et Technologies, USR 3290 MSAP, Miniaturisation pour l'Analyse, la Synthèse et la Protéomique, 59655 Villeneuve d'Ascq Cedex, France, Villeneuve D'ascq Cedex, France; [2]Université de Rouen, UMR 6014, CNRS, COBRA, Chimie organique et bioorganique, Réactivité et Analyse, 76821 Mont-Saint-Aignan Cedex, France, Rouen, France; [3]Muséum National d'Histoire Naturelle, USR 3224, CNRS, Centre de Recherche sur la Conservation, 36, rue Geoffroy Saint-Hilaire, 75005 Paris, Paris, France*

ThOG pm 03:50 **Empty Slot.** Stay tuned for promoted selection to be made.

ThOG pm 04:10 **Empty Slot.** Stay tuned for promoted selection to be made.

ThOH pm: Fundamentals for Everyone: Imaging

Chair: Nathalie Agar (Harvard University)

ThOH pm 02:30 **Exploratory and Predictive Analysis of Imaging MS Data: Machine Learning Approaches**; Raf Van de Plas[1, 2, 3]; Lukasz G. Migas[1]; Leonoor E.M. Tideman[1]; Emilio S. Rivera[2, 3]; Katerina V. Djambazova[2, 4]; Elizabeth K. Neumann[2, 3]; N. Heath Patterson[2, 3]; Jeffrey M. Spraggins[2, 3, 4]; Richard M. Caprioli[2, 3, 4, 5, 6]; [1]*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN*

ThOH pm 02:50 **Performance Evaluation of a MALDI LTQ Orbitrap XL Imaging Platform Interfaced with a New-Generation Data Acquisition System**; Konstantin O. Nagornov[1]; Anton N. Kozhinov[1]; Franklin E. Leach III[2]; Yury O. Tsybin[1]; [1]*Spectroswiss, Lausanne, Switzerland; [2]University of Georgia, Athens, GA*

ThOH pm 03:10 **Measuring spatial resolution in Mass Spectrometry Imaging – development of parametric and non-parametric approaches**; Martin Metodiev[1, 2]; Rory T Steven[1]; Xavier Loizeau[1]; Alex Dexter[1]; Chelsea Nikula[1]; Ammar Nasif[1]; Kenneth Robinson[1]; Bin Yan[1]; Zoltan Takats[2]; Josephine Bunch[1, 2]; [1]*NPL, Teddington, United Kingdom; [2]Imperial College London, london, United Kingdom*

ThOH pm 03:30 **Tandem mass tag labeling enables high throughput imaging of 2000 proteins at 50-μm spatial resolution from tissue sections**; Ying Zhu[1]; Paul D Piehowski[1]; Yang Wang[1]; Kelly G Stratton[1]; Sarah M. Williams[1]; Jia Yuan[2]; Sudhansu K Dey[2]; Ronald J. Moore[1]; Richard D. Smith[1]; Lisa M Bramer[1]; Kristin E Burnum-Johnson[1]; [1]*Pacific Northwest National Laboratory, Richland, WA; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

ThOH pm 03:50 **Discovering powerful biocatalysts with a novel platform combing microdroplet-printing and microscale mass spectrometry imaging**; Linfeng Xu[1]; Leqian Liu[1]; Adam Abate[1, 2]; Nannan Tao[3]; Shannon Cornett[4]; [1]*University of California San Francisco, San Francisco, CA; [2]Chan Zuckerber Biohub, San Francisco, CA; [3]Bruker Scientific, San Jose, CA; [4]Bruker Scientific LLC, Billerica, MA*

ThOH pm 04:10 **Development of an Instrument Optimized for Multiplexed Ion Beam Imaging of 2D Tissue Samples**; Elizabeth R Schemm[1]; Ben Shepperson[1]; Jay G Tarolli[1]; Steve P Thompson[1]; Rich Tighe[1]; [1]*IONpath, Menlo Park, CA*

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AMBIENT IONIZATION: APPLICATIONS I
MP 001-027

MP 001 **A Real Time Metabolomic Profiling Approach to Authentication of Ginkgo Biloba Extracts Products Using Rapid Evaporative Ionization Mass Spectrometry**; Yisheng Xu[1, 2]; Jinghui Wang[1, 3]; Shuang Fang[1, 2]; Kate Yu[2]; Jihong Lin[2]; Hongzhu Guo[3]; Zhongzhi Qian[1]; *[1]Chinese Pharmacopeia/Waters Joint Open Lab, Beijing, China; [2]Waters cooperation, Shanghai, China; [3]Beijing Institute for Drug Control, Beijing Key Laboratory of Analysis and Evaluation on Chinese Medicine, Beijing, China*

MP 002 **PiTMaP: a new analytical platform for high-throughput direct metabolome analysis using PESI/MS/MS with the R software-based data pipeline**; Kei Zaitsu[1, 2]; Seiichiro Eguchi[3]; Tomomi Ohara[2]; Akira Ishii[2]; Takakazu Kawamata[3]; Akira Iguchi[4]; *[1]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [2]Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]Department of Neurosurgery, Tokyo Women's Medical University, Tokyo, Japan; [4]Marine Geo-Environment Research Group, Institute of Geology and Geoinformation, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan*

MP 003 **High-throughput and sensitive analysis of diverse molecules using AP MALDI interfaced with a QqTOF system**; Vishal Mahale[1]; Dipankar Malakar[2]; Rashid Faraz[3]; Dharmeshkumar Parmar[4, 5]; Subodh Chawan[6]; Venkateswarlu Panchagnula[1, 4, 5]; *[1]Barefeet Analytics Pvt. Ltd., Pune, India; [2]AB Sciex, India, Gurgaon, India; [3]AB Sciex, India, Gurgaon, India; [4]CSIR-National Chemical Laboratory, Pune, India, Pune, India; [5]Academy of Scientific and Innovative Research (AcSIR), Pune, India; [6]Scientia Life Technologies LLP, Mumbai, India*

MP 004 **Rapid Flux Phenotyping by DESI-Ion Mobility-Imaging Mass Spectrometry to Accelerate Metabolic Engineering of Bacteria**; Berkley Ellis[1]; Piyoosh Babele[1]; Jody C. May[2]; Brian Pfleger[3]; Jamey Young[2]; John A. McLean[2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt Unviersity, Nashville, TN; [3]University of Wisconsin, Madison, WI*

MP 005 **Versatile (applications with) metalspray in mass spectrometry using hydrophobic/omniohobic surfaces**; Michael C Godwin[1]; William Hoffmann[1]; *[1]Texas State University, San Marcos, TX*

MP 006 **Python-powered kinetic analysis of data rich mass spectrometric reaction monitoring**; Sofia Donnecke[1]; Brett Henderson[2]; Scott Mcindoe[2]; *[1]University of Victoria, Victoria, BC; [2]University of Victoria, Victoria, British Columbia*

MP 007 **Analysis of Cholesterol and Androgens in Mouse Prostate Cells by LC-MS/MS: HESI versus APCI**; Min Liu[1]; Jayden K. Cline[1]; Asmaa Elkenawi[1]; Brian Ruffell[1]; John M. Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL*

MP 008 **Contained-Electrospray Ionization to Study Accelerated Lipid Hydrolysis by Lipase Enzyme in Aerosol Proxies**; Benjamin J Burris; *The Ohio State University, Columbus, OH*

MP 009 **Coated Blade Spray-Tandem Mass Spectrometry for Rapid Screening and Quantitation of target drugs in Oral Fluids and Plasma Samples**; Shane Stevens[1]; German Augusto Gomez-Rios[1]; Gary Stidsen[1]; David S. Bell[1]; *[1]Restek Corporation, Bellefonte, PA*

MP 010 **Software tool for visual inspection of the stability and reproducibility of mass spectra**; Evgeny Zhvansky[1]; Anatoly Sorokin[1]; Daniil Ivanov[1]; Denis Zavorotnyuk[1]; Stanislav Pekov[1]; Vasiliy Eliferov[1]; Eugene (evgeny) Nikolaev[2]; Igor Popov[1]; *[1]Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 011 **Low ion suppression in optimized coated blade spray for complex samples: Result of good sample preparation prior to ambient ionization**; Abir Khaled[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON*

MP 012 **High-throughput Determination of Pesticides using DART-QTOF MS**; Wei Du*[1]; Wei Chen[2]; Kerry Song[2]; Xiaokun Duan[2]; *[1]Agilent Technologies, Beijing, China; [2]ASPEC Technologies, Beijing, China*

MP 013 **Reactive Flowing Atmospheric Pressure Afterglow for Derivatization Analytes in Real-time.**; Dong Zhang[1]; Maureen Oliva[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 014 **Modified Conical Ablation Chamber for Remote Laser Ablation Electrospray Ionization Mass Spectrometry**; Marjan Dolatmoradi[1]; Jarod A. Fincher[1]; Andrew R. Korte[1]; Nicholas J. Morris[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Air Force Research Laboratory, Dayton, OH*

MP 015 **Integrating Desorption Electrospray Ionization Mass Spectrometry Imaging and Fluorescence In-Situ Hybridization for the Detection of Circulating Tumor Cells**; Alena Bensussan[1]; Tanweer Zaidi[2]; Ruth Katz[2]; Livia S. Eberlin[1]; *[1]The University of Texas at Austin, Austin, TX; [2]MD Anderson, Houston, TX*

MP 016 **Solid Phase Microextraction Probe Electrospray Ionization for Quantitation of Drugs of Abuse in Small Volumes of Plasma**; Milaan Thirukumaran[1]; Varoon Singh[1]; Yohei Arao[2]; Yuka Fujito[2]; Masayuki Nishimura[2]; Hidekazu Saiki[3]; Yoshihiro Hayakawa[3]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD; [3]Shimadzu Corporation, Kyoto, Japan*

MP 017 **Capturing Fleeting Intermediates in Uncatalyzed Claisen Rearrangement under Non-Equilibrium Droplet Imbibition Conditions**; Taghi Sahraeian[1]; Abraham K. Badu-Tawiah[1]; [1]*The Ohio State University, Columbus, OH*

MP 018 **Dual desorption electrospray ionization and laser mass spectrometry imaging using the same interface**; Lauren H Katz[1]; Michael Woolman[1]; Francis Talbot[1]; Siham Amara-Belgadi[1]; Megan Wu[2]; Sara Tortorella[3]; Sunit Das[2]; Howard Ginsberg[4]; Arash Zarrine-Afsar[1]; [1]*University of Toronto, Toronto, Ontario; [2]Peter Gilgan Centre for Research and Learning, Hospital for Sick Children, Toronto, Ontario; [3]Molecular Horizon, Bettona, Italy; [4]St. Michael's Hospital, Toronto, Ontario*

MP 019 **Studies of reaction acceleration in microdroplets, thin films and sealed microchannels**; Lingqi Qiu[1]; Zhenwei Wei[1]; Honggang Nie[1, 2]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN; [2]Peking University, Haidian, China*

MP 020 **Serine Enhances Protein Analysis by DESI-MS**; Roshan Javanshad[1]; Andre R Venter[1]; [1]*Western Michigan University, Kalamazoo, MI*

MP 021 **High-yield gram-scale organic synthesis using solvent recycling accelerated microdroplet/thin film reactor**; Honggang Nie[1, 2]; Zhenwei Wei[1]; Lingqi Qiu[1]; Xingshuo Chen[1]; Dylan T. Holden[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN; [2]Peking University, College of Chemistry, Beijing, China*

MP 022 **Monitoring peppermint washout in the breath metabolome by secondary electrospray ionization-high resolution mass spectrometry**; Jiayi Lan[1]; Renato Zenobi[1]; [1]*ETH Zurich, Zurich, Switzerland*

MP 023 **Rapid evaporative ionisation mass spectrometry and direct analysis in real time-mass spectrometry as techniques to rapidly determine poultry meat characteristics**; Nicholas Birse[1]; Olivier Chevallier[2]; Sara Stead[3]; Steven Pringle[3]; Vit Kosek[4]; Vojtech Hrbek[4]; Jana Hajslov[4]; Christopher Elliot[1]; [1]*Institute for Global Food Security, Queen's University Belfast, Belfast, United Kingdom; [2]Mass Spectrometry Core Technology Unit, Queen's University Belfast, Belfast, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom; [4]University of Chemistry and Technology, Prague, Czech Republic*

MP 024 **Reaction Acceleration at Air-Solution Interfaces: Anisotropic Rate Constants for Katritzky Transamination**; Yangjie Li[1]; Tsdale F. Mehari[1]; Zhenwei Wei[1]; Yong Liu[2]; R. Graham Cooks[1]; [1]*Purdue University, Lafayette, IN; [2]Merck & Co., Rahway, NJ*

MP 025 **Rapid Quantitative Screening of Cyanobacteria for Anatoxins Using Direct Analysis in Real Time-High Resolution Mass Spectrometry**; Daniel Beach[1]; Cheryl Rafuse[1]; Jeremy E. Melanson[2]; Pearse Mccarron[1]; [1]*Biotoxin Metrology, National Research Council Canada, Halifax, NS; [2]Organic Chemical Metrology, National Research Council Canada, Halifax, NS*

MP 026 **Analysis of Oceanic Systems by TM-DART-QTOF-MS-Based Seaomics**; Nicolas Zabalegui[1]; Malena Manzi[1]; Antoine Depoorter[2]; Nathalie Hayeck[2]; Marie Roveretto[2]; Chunlin Li[2, 3]; Manuela Van Pinxteren[4]; Hermann Hartmut[4]; Christian George[2]; Maria Eugenia Monge[1]; [1]*Centro de Investigaciones en Bionanociencias (CIBION), CONICET, Buenos Aires, Argentina; [2]Université de Lyon 1, CNRS, IRCELYON, Villeurbanne, France; [3]Weizmann Institute of Science, Rehovot, Israel; [4]Leibniz-Institut für Troposphärenforschung e.V., Leipzig, Germany*

MP 027 **In vivo mapping of cell type-specific interactome study in mouse brain**; Xiaojun Sun[1]; Xian Han[1]; Huan Sun[2]; Ping-Chung Chen[1]; Yun Jiao[1]; Junmin Peng[1]; [1]*St jude Children's research hospital, Memphis, TN; [2]St. Jude Children's research hospital, Memphis, TN*

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION
MP 028-047

MP 028 **Detection of Chemical residues, Metabolites and Gaseous capture utilizing a Microporous Polyolefin Silica-based Substrate for Paper Spray Mass Spectrometry**; Imesha G. Weligamage De Silva[1]; Thomas D Kiselak[1]; Alleigh Nicole Couch[1]; Cristina Castillo[1]; Guido F. Verbeck[1]; [1]*University of North Texas, Denton, TX*

MP 029 **Expanding the Applications of Laser-Assisted Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS) to the Pharmaceutical Product Development Workflow**; Toma Ramonaite[1]; Alvaro Perdones-Montero[1]; Andrew Ray[2]; Miriam Guest[2]; Simon Cameron[1]; Zoltan Takats[1]; [1]*Imperial College London, London, United Kingdom; [2]AstraZeneca, Macclesfield, United Kingdom*

MP 030 **Programmed Droplet Desolvation And Occam's Razor**; Drew Sauter[1]; Andrew D Sauter III[1]; Ron Shomo[2]; [1]*Nanoliter, LLC, Henderson, NV; [2]Adaptas, Palmer, MA, Massachusetts*

MP 031 **Non-proximate Ambient Sampling for Solvent-free Analysis of Intact Objects**; G. Asher Newsome[1]; Kathleen Martin[2]; Julia Campbell-Such[3]; [1]*Smithsonian Museum Conservation Institute, Suitland, MD; [2]Smithsonian National Museum of the American Indian, Hillcrest Heights, MD; [3]Smithsonian National Museum of African Art, Washington, DC*

MP 032 **Counterions for Ambient Ion Focusing**; Saquib Rahman[1]; Brett M. Marsh[1]; Shane Tichy[2]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN; [2]Agilent Technologies, Santa Clara, CA*

MP 033   **Condensed Liquid Aerosol Particle Spray (CLAPS) Coupled to MS – a Novel On-Line Liquid Aerosol Analysis Technique**; <u>Nathaneal A Park</u>[1]; Spencer E Tilley[1]; Gary L Glish[1]; [1]*UNC Chapel Hill, Chapel Hill, NC*

MP 034   **Quantitation with Direct Analysis in Real Time Mass Spectrometry by utilizing less sample**; <u>Paul Liang</u>[1]; Frederick Li[1]; Brittany Laramee[1]; Brian Musselman[1]; [1]*IonSense,Inc., Saugus, MA*

MP 035   **An Integrated Microfluidic probe for High-Resolution and High-throughputNano-DESI Mass Spectrometry Imaging of Tissue Sections**; <u>Xiangtang Li</u>[1]; Ruichuan Yin[1]; Julia Laskin[1]; [1]*Purdue University, West Lafayette*

MP 036   **Serine sublimation: from racemic crystal to homochiral octamer in gas phase**; <u>Rong Chen</u>[1]; Zhenwei Wei[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN*

MP 037   **Combined Mechanospray Ionization with a Discharge Needle Shifts Charge State Distributions in Real-Time**; <u>Liam Dugan</u>[1]; Mark E Bier[1]; [1]*Carnegie Mellon University, Pittsburgh, PA*

MP 038   **Spatially Resolved Chemical Profiling of Porous Membrane Flow Cell Content via Droplet-Based Liquid Microjunction Surface Sampling Probe-HPLC-ESI-MS**; <u>Vilmos Kertesz</u>[1]; John F. Cahill[1]; Scott T. Retterer[1]; Muneeba Khalid[1]; Courtney L. Walton[1]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN*

MP 039   **Novel Systems and Methods for Picoflow Electrospray**; Mengtian Li[1]; Linfan Li Li[2]; Jae Schwartz[2]; <u>Anyin Li</u>[1]; [1]*University of New Hampshire, Durham, NH;* [2]*Thermo Fisher Scientific, San Jose, CA*

MP 040   **Investigating Molecular Extraction and Ionization Processes in Solvent-Based Ambient Ionization Mass Spectrometry**; <u>Monica Lin</u>[1]; Molly S. Blevins[1]; Marta Sans[1]; Jennifer S. Brodbelt[1]; Livia S. Eberlin[1]; [1]*University of Texas at Austin, Austin, TX*

MP 041   **Hybrid thermal desorption – ambient mass spectrometry developments for the trace detection of explosives, illicit narcotics, and related species**; <u>Thomas P. Forbes</u>[1]; Edward Sisco[1]; Matthew Staymates[1]; [1]*National Institute of Standards and Technology, Gaithersburg, MD*

MP 042   **Integration of 3D Printing into Desorption Electrospray Ionization Mass Spectrometry**; <u>Kevin J Zemaitis</u>[1]; Kathiravan Kaliyappan[1]; Vp Krishnan Muthaiah[1]; Alexis C Thompson[1]; Troy D Wood[1]; [1]*University at Buffalo, Buffalo, NY*

MP 043   **Cone-jet mode electrospray Ionization in microflow and nanoflow regimes by emitter surface manipulations**; <u>Sau Lan Staats</u>[1]; Anna Stoltzfus[1]; Andris Suna[1]; [1]*Phoenix S & T, Inc, Chadds Ford, PA*

MP 044   **Rapid Screening and Confirmation of target analytes in biological fluids using a single sample and a single sampling collection device**; <u>German Augusto Gómez-Ríos</u>[1]; Shane Stevens[1]; David S. Bell[1]; Gary Stidsen[1]; [1]*Restek Corporation, Bellefonte, PA*

MP 045   **Nanometer Scale Chemical and Functionals Imaging on an AFM-MS System**; Ryan Wagner[1]; Matthias Lorenz[2, 3]; Olga S. Ovchinnikova[3]; <u>Roger Proksch</u>[1]; [1]*Oxford Instruments, Goleta, CA;* [2]*University of Tennessee Knoxville, Knoxville, TN;* [3]*Oak Ridge National Laboratory (ORNL), Oak Ridge, TN*

MP 046   **Implementation of marker tips for touch spray ionization**; Roman Levin[1]; Denis Bormotov[1, 2]; Konstantin Bocharov[1, 2]; Anna Mishina[1]; <u>Vsevolod Shurkhay</u>[1]; Stanislav Pekov[1, 2]; Eugene (evgeny) Nikolaev[3]; Igor Popov[1]; [1]*Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation;* [2]*V.L. Talrose Institute for Energy Problems of Chemical Physics, N.N. Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, Moscow, Russia;* [3]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 047   **Application of a non-fixed magnetic carbon nanotube paper in paper spray analysis**; <u>Tássia Venga Mendes Venga Mendes</u>[1]; Eduardo Costa De Figueiredo[2]; Nicholas E. Manicke[1]; [1]*Indiana University Purdue University Indianapolis, Indianapolis, IN;* [2]*Federal University of Alfenas, Alfenas, Brazil*

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
MP 048-065

MP 048   **Site specific glycan profiling of N-glycans from Cetuximab**; Min Kyung So[1]; Chung Su Lim[1]; Ju Hyeon Lim[1]; In Young Ko[1]; Ah Young Ki[1]; <u>Byoung Joon Ko</u>[1]; [1]*Kbiohealth, Cheonju-si, South Korea*

MP 049   **Distinguishing of isomeric Leu/Ile residues by Integrated LC-hot ECD MS/MS in an RF Ion Trap**; <u>Khadijeh Rajabi</u>[1]; Takashi Baba[1]; [1]*SCIEX, Concord, ON*

MP 050   **Study of glycosylation in Monoclonal Antibody using Intact and Middle-Down Approach**; <u>Keqin Chen</u>[1]; Takashi Baba[1]; [1]*SCIEX, Concord, ON*

MP 051   **IdeS on magnetic beads enables parallel and automated antibody subunit generation for rapid middle-level MS analysis of critical quality attributes**; <u>Hanna Toftevall</u>[1]; Philip J. Widdowson[2]; Andreas Nägeli[1]; Helén Nyhlén[1]; Fredrik Olsson[1]; [1]*Genovis AB, Lund, Sweden;* [2]*Thermo Fisher Scientific, Runcorn, United Kingdom*

MP 052   **Offline IEX fractionation of monoclonal antibodies enhances coverage of proteoforms in native CZE-MS analysis**; <u>Kendall Johnson</u>[1]; Erica Teng[1]; Marcia Santos[2]; Alexander R. Ivanov[1]; [1]*Northeastern University, Boston, MA;* [2]*Sciex, Brea, CA*

MP 053 **Comprehensive Characterization of Monoclonal Antibody and Antibody Drug Conjugate on a Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Kristina Srzentic[1]; Eugen Damoc[2]; Angela Criscuolo[3]; Tom Buchanan[4]; Krisztina Radi[5]; Marc Guender[6]; [1]*Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Dreieich, Germany; [4]Thermo Fisher Scientific, Runcorn, United Kingdom; [5]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [6]Thermo Fisher Scientific, reinach, Switzerland*

MP 055 **Characterization of O-glycosylation by mass spectrometry to support process development of an Fc-fusion protein**; Renpeng Liu[1]; Rachel Chen[1]; Zoran Sosic[1]; [1]*Biogen, Cambridge, MA*

MP 056 **Characterization and comparison of Neulasta and its biosimilar at intact level on a quadrupole-Orbitrap mass spectrometer**; Xiaoxi Zhang[1]; Haichuan Liu[2]; Hao Yang[2]; Min Du[3]; [1]*ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, San Jose, California; [3]ThermoFisher Scientific, Massachusetts, Massachusetts*

MP 057 **TSPR-MS: New Online Epitope Analyzer for Epitope and Affinity Determination of Antibody- Ligand Interactions**; Frederik Barka[1]; Loredana Lupu[2]; Pascal Wiegand[2]; Delia Mihoc[2]; Oliver Mueller[2]; Friedemann Voelklein[3]; Guenes Barka[1]; Michael Przybylski[2]; [1]*Sunchrom GmbH, Friedrichsdorf, Germany; [2]Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spec, Ruesselsheim, Germany; [3]Rhein Main University, Ruesselsheim, Germany*

MP 058 **Free Thiol Quantification of Antibodies and Cysteine-Conjugated Antibody Drug Conjugates by Maleimide-Labeling and Intact Mass Analysis**; Benjamin Cutak[1]; Ken Chanthamontri[1]; Kevin Ray[1]; [1]*MilliporeSigma, St. Louis, MO*

MP 059 **Linking Biochemical and Biophysical Antibody Drug Conjugate (ADC) Data in Assessing Drug-to-Antibody Ratio (DAR)**; Colette Quinn[1]; Henry Shion[2]; [1]*Waters Corporation, Milford, Massachusetts; [2]Waters Technologies Corporation, Milford, MA*

MP 060 **Rapid microfluidic method for molecular weight determination and spent media analysis of an IgG1 intact protein in growth media**; Adi M Kulkarni[1]; Kenion H Blakeman[1]; Kathryn Elliott[2]; Colin M Gavin[1]; Ji Young L Anderson[1]; Sarah Harcum[2]; Glenn A Harris[1]; [1]*908 Devices, Inc., Boston, MA; [2]Clemson Univ., Dept. of Bioengineering, Clemson, SC*

MP 061 **Innovative LCMS platform for Antibody Drug Conjugate (ADC) Characterization under Native Conditions: Drug-to-Antibody Ratio (DAR) distribution monitoring in biological samples**; Shuai Niu[1]; Daniel Ladror[1]; Gary Jenkins[1]; John Paul Savaryn[1]; [1]*AbbVie Inc, North Chicago, IL*

MP 062 **Combination of Hybrid LC-MS and HR-MS Techniques to Characterize Uncialamycin Antibody Drug Conjugates**; Jose Trinidad[1]; Amanda Valdiosera[1]; Hetal Sarvaiya[1]; Christine Gu[1]; Julia Gavrilyuk[1]; Beth Pysz[1]; [1]*Abbvie South San Francisco, South San Francisco, CA*

MP 063 **Assessing oxidation of methionine in a cysteine-conjugated ADC by affinity capture subunit liquid chromatography-mass spectrometry analysis**; Wen Zhang[1]; Tong Ding[1]; Samir Das[1]; Andrea Hernandez[1]; Jodi Wong[1]; Dunja Urosev[1]; Jamie Rich[1]; [1]*Zymeworks Inc., Vancouver, BC*

MP 064 **TArget-Responsive SubCellular Pharmacokinetics for Early-stage Antibody-Drug Conjugates Screening and Assessment**; Jiali Liu[1]; Hua Sang[2]; Xiaofang Zhang[1]; Ning Wang[1]; Yazhong Liu[1]; Guangji Wang[1]; Hui Ye[1]; [1]*China Pharmaceutical University, Nanjing, China; [2]Department of Pharmacy, The Affiliated Hospital of Nantong University, Nantong, China*

MP 065 **Discovery of photoinduced cross-links in monoclonal antibodies**; Thomas Powell[1]; Michael Knight[1]; John O'hara[1]; William Burkitt[1]; [1]*UCB, Slough, United Kingdom*

**CANNABIS
MP 066-083**

MP 066 **Analysis of Tetrahydrocannabinol Vape Oils Using Pyrolyzer**; Karen Sam[1]; Ben Landas[1]; [1]*CDS Analytical, Oxford, PA*

MP 067 **MALDI-MS Library of Fingerprint Spectra for Selected Fractions of Cannabis Products**; Baylie Gigolyk[1]; Helene Perreault[1]; [1]*University of Manitoba, Winnipeg, MB*

MP 068 **Methodology for Targeted and Non-Targeted Screening and Differentiation of Cannabis Cultivars**; Marian Twohig[1]; Steven Lai[1]; Angus Black[2]; Christopher Hudalla[3]; Justin Chang[1]; Kenneth Rosnack[1]; [1]*Waters Corporation, Milford, MA; [2]Nonlinear Dynamics, Newcastle upon Tyne, United Kingdom; [3]Proverde Laboratories, Milford, MA*

MP 069 **Developing Cannabis Chemovar Maps using Comprehensive Two-Dimensional Gas Chromatography with High-Performance Time-of-Flight Mass Spectrometry (GCxGC-TOFMS)**; David E Alonso[1]; Elizabeth Humston-Fulmer[1]; Christina Kelly[1]; Joe Binkley[1]; [1]*Leco Corporation, St. Joseph, MI*

MP 070   **Detection of typical GCMS Pesticides in Cannabis Matrix utilizing APCI-LCMS**; <u>Jennifer C Davis</u>[1]; Evelyn H Wang[2]; Katie Pryor[2]; Priyanka Chitranshi[2]; Christopher T. Gilles[2]; *[1]Shimadzu Scientific Inc., Columbia, MD; [2]Shimadzu Scientific Instruments Inc., Columbia, MD*

MP 071   **ICP-MS Analysis of Cannabis Sativa Using Novel US State Specific CRM Heavy Metal Mixes (As, Cd, Hg and Pb)**; <u>Stephan Altmaier</u>; *Merck KGaA, Darmstadt, Germany*

MP 072   **Method development for pesticides analysis in cannabis oil**; <u>Xuejun Zang</u>[1]; Asha A. Oroskar[1]; Anil Oroskar[1]; *[1]Orochem Technologies Inc, Naperville, IL*

MP 073   **An in-depth evaluation of accuracy in cannabis potency testing methods**; <u>Zachary Kelley</u>[1]; Bert C. Lynn[1]; *[1]Department of Chemistry, University of Kentucky, Lexington, KY*

MP 074   **Developing a discovery-based approach to cannabis testing using GC×GC-TOF MS**; Laura Mcgregor[1]; Bob Green[1]; Matthew Edwards[2]; David Bowman[2]; Wade Bontempo[3]; <u>Kevin Kyle</u>[3]; *[1]SepSolve Analytical, Peterborough, United Kingdom; [2]SepSolve Analytical, Waterloo, ON; [3]Markes International Inc, Sacramento, CA*

MP 075   **QUALITATIVE/ QUANTITATIVE ANALYSIS OF A METABOLIC PATHWAY IN POPULAR CBD BEVERAGES & OILS USING GC-MS & UHPLC-HRMS**; <u>Eloisa Franco</u>[1]; Vedanga Arekar[1]; Maria Alejo-Diaz[1]; Sneha Kadam[1]; Dil Ramanathan[1]; *[1]Kean University, Union, NJ*

MP 076   **Comparative Analysis of Kava and Industrial Hemp Using GC-MS**; <u>Dhara Patel</u>[1]; Daniel George[2]; Sneha Kadam[1]; Eloisa Franco[1]; Yuriko Root[1]; Dil Ramanathan[1]; *[1]Kean University, Union, NJ; [2]Ridge High School, Basking Ridge, NJ 07920*

MP 077   **Fast Quantitative Analysis of major and minor Cannabinoids in Hemp using LC-MSMS method with single sample dilution and injection**; <u>Avinash Dalmia</u>[1]; Saba Hariri[2]; Jacob Jalali[3]; Feng Qin[2]; Thomas White[4]; *[1]Perkinelmer, Shelton, CT; [2]Perkin Elmer, Wood bridge, ON; [3]PerkinElmer, Inc., San Jose, CA; [4]PerkinElmer, Shelton, CT*

MP 078   **A Fast, Sensitive and Comprehensive Assay to Quantify 16 Cannabinoids in Hemp Plant using LC/MS/MS**; <u>Aihua Liu</u>[1]; Daniel Taylor[1]; Amy Wei[1]; Spencer Carter[1]; *[1]Dyad Labs, Salt Lake City, UT*

MP 080   **Analysis of the California list of pesticides and mycotoxins in cannabis edibles**; <u>Nathaly Reyes Garces</u>[1]; Colton Myers[1]; Ashlee Gerardi[1]; *[1]Restek Corporation, Bellefonte, PA*

MP 081   **Future-proofing Cannabis analysis with a hybrid triple quadrupole/linear ion trap system**; Katherine Hyland[1]; <u>Robert Di Lorenzo</u>[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ontario*

MP 082   **Analytical Workflows Using Orbitrap Mass Spectrometry to Evaluate Potency in Cannabis-Containing Edibles**; <u>Ryan Hayward</u>[1]; Rob O'brien[1, 2]; Matthew Noestheden[1, 2]; *[1]Supra R&D, Kelowna, BC; [2]University of British Columbia, Kelowna, BC*

MP 083   **Development of a Robust LC-MS/MS Method for the Simultaneous Quantification of Cannabidiol (CBD), Tetrahydrocannabinol (THC) and their Metabolites in Plasma**; <u>Mays Al-Dulaymi</u>[1]; Christine Allen[1]; *[1]Leslie Dan Faculty of Pharmacy, University of Toronto, Toronto, ON*

CARBOHYDRATES I
MP 084-100

MP 084   **Structural determination of polysaccharides using logically derived sequence tandem mass spectrometry**; <u>Chi-Kung Ni</u>; *Academia Sinica, Taipei, Taiwan*

MP 085   **Sialylation Status and Mechanical Properties of THP-1 Macrophages Upon LPS Stimulation**; <u>Yu Zhao</u>[1]; Gautam Mahajan[1]; Chandrasekhar Kothapalli[1]; Xue-Long Sun[1]; *[1]Cleveland State University, Cleveland, OH*

MP 086   **Monitoring Oligosaccharides From Glycosyltransferase Reactions Using Paper Spray Mass Spectrometry (PS-MS)**; <u>Qi Wang</u>[1]; Pengyi Zhao[1]; Matrika Bhattarai[2]; Michael Held[2]; Ahmed Faik[2]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Ohio University, Athens, OH*

MP 087   **Towards a more complete glycome: advances in ion chromatography-mass spectrometry (IC-MS) for improved separation and analysis of carbohydrates**; <u>Neil Gregory Rumachik</u>; *Thermo Fisher Scientific, Sunnyvale, CA*

MP 088   **Structural Characterization of Glycans by Electron-Transfer/Higher-Energy Collision Dissociation**; <u>Tengfei Yuan</u>[1, 2]; Juan Wei[1]; Yang Tang[1, 3]; Catherine E Costello[1, 3]; Cheng Lin[1]; *[1]Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; [2]Department of Clinical Laboratory, Renmin Hospital of Wuhan University, Wuhan, China; [3]Department of Chemistry, Boston University, Boston, MA*

MP 089   **N-glycan profiling of kidney brush border membrane from rats using LC-MS/MS analysis**; <u>Aiying Yu</u>[1]; Jingfu Zhao[1]; Bruce A. Molitoris[2]; Mark C. Wagner[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Indiana University, Indianapolis, IN*

MP 090   **Parallel reaction monitoring study of micro-heterogeneity of haptoglobin from human blood serum**; Cristian D Gutierrez Reyes[1]; Yifan Huang[1]; Mojgan Atashi[1]; Jianhui Zhu[2]; David M Lubman[2]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX;* [2]*University of Michigan, Ann Arbor, MI*

MP 091   **Carbohydrate Characterization of Traditional Chinese Medicine Using Rapid High-Throughout Mass Spectrometry-Based Methods**; Ye Chen[1]; Juan J Castillo[1]; Eshani Nandita[2]; Garret Couture[1]; Carlito B Lebrilla[1]; [1]*University of California, Davis, Davis, CA;* [2]*Emery Pharma, Alameda, CA*

MP 092   **Negative Ion Mode Electron Capture Dissociation of Synthetic Heparan Sulfate Oligosaccharides**; Isaac Agyekum[1]; Adrian Kim[1]; Lauren Pepi[2]; Jonathan I Amster[2]; [1]*University of North Georgia - Gainesville Campus, Oakwood GA, Georgia;* [2]*University of Georgia, Athens, GA*

MP 093   **Identification of Synthetic Heparan Sulfate Glycosaminoglycan Hexasaccharides Epimers by Capillary Zone Electrophoresis Negative Electron Transfer Dissociation Tandem Mass Spectrometry**; Marshall Liss[1]; Lauren E. Pepi[1]; Pradeep Chopra[1]; Geert-Jan Boons[1]; Jon Amster[1]; [1]*University of Georgia, Athens, GA*

MP 094   **Three-plexed Quantification of Glycans in Yeast using Metabolic Isotope Labeling by Mass Spectrometry**; Jae-Min Lim[1]; Thao Thi Pham[1]; Jihee Yoon[1]; [1]*Changwon National University, Changwon, South Korea*

MP 095   **Study of cnidarian-dinoflagellate symbiosis by analysis of cell surface N-glycans in dinoflagellate symbionts**; Xue Dong[1]; Wenjing Peng[1]; Trevor R. Tivey[2]; John Everett Parkinson[2, 3]; Paige E. Mandelare[2, 4]; Donovon A. Adpressa[2]; Virginia M. Weis[2]; Sandra Loesgen[2, 4]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX;* [2]*Oregon State University, Corvallis, OR;* [3]*University of South Florida, Tampa, FL;* [4]*University of Florida, St. Augustine, FL*

MP 096   **Quantum Chemical Calculations for Mechanistic Study of Free Radical Activated Glycan Dissociation through 13C-Labeled Cellobioses**; Rose Mery Bakestani[1]; Hendrik Eshuis[1]; Jinshan Gao[1]; [1]*Montclair State University, Upper Montclair, NJ*

MP 097   **Glycosidic bond position of linear oligosaccharides using the cross-ring fragments produced by helium-charge transfer dissociation mass spectrometry**; Hagen Buck-Wiese[1, 2]; Mathieu Fanuel[3]; Manuel Liebeke[1]; Jan-Hendrik Hehemann[1, 2]; Hélène Rogniaux[3]; Glen P. Jackson[4]; David Ropartz[3]; [1]*Max-Planck-Institute for marine microbiology, Bremen, Germany;* [2]*Marum Center for Marine Environmental Sciences, Bremen, Germany;* [3]*INRAE, BIBS facility, Nantes, France;* [4]*West Virginia University, Morgantown*

MP 098   **Structural Characterization of a Mixture of Complex Sulfated Oligosaccharides Using Ultra-High Performance Liquid Chromatography with Charge Transfer Dissociation Mass Spectrometry**; Praneeth M Mendis[1]; Zachary J. Sasiene[1]; David Ropartz[2]; Hélène Rogniaux[2]; Glen P. Jackson[1, 3]; [1]*C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV;* [2]*INRAE, UR BIA, Nantes, France;* [3]*Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

MP 099   **Combining cryogenic infrared spectroscopy with selective enzymatic cleavage for determining glycan primary structure**; Irina Dyukova[1]; Eduardo Carrascosa[1]; Robert P Pellegrinelli[1]; Thomas R. Rizzo[1]; [1]*EPFL/LCPM, Lausanne, Switzerland*

MP 100   **N-glycosylation profiling of a biotherapeutic protein by combining ultrahigh-resolution ion mobility spectrometry and cryogenic ion spectroscopy**; Natalia Yalovenko[1]; Vasyl Yatsyna[1]; Priyanka Bansal[1]; Ali H Abikhodr[1]; Thomas R. Rizzo[1]; [1]*EPFL/LCPM, Lausanne, Switzerland*

CORPORATE POSTERS I
MP 101-103

MP 101   **Bruker at ASMS 2020: MALDI II for dramatic sensitivity improvements in SpatialOMx workflows, Bruker Daltonics**

MP 102   **Analytical Intelligence in the Digital Age of Mass Spectrometry, Shimadzu Scientific Instruments**

MP 103   **Orbitrap Exploris Mass Spectrometry, Thermo Fisher Scientific**

DDA AND DIA LC-MS: FUNDAMENTALS
MP 104-107

MP 104   **The development of curved LC gradient methodfor analyzing complex mixture by high-resolution hybrid mass spectrometer**; Leila Afjehi; *University of Vienna, Vienna, Austria*

MP 105   **Development of DDA and DIA analysis pipeline for the study of insulin resistance in human liver samples**; Mauro Galli[1]; Hady Razak Hady[2]; Lukasz Szczerbinski[3]; Agnieszka U. Blachnio-Zabielska[4]; Adam Kretowski[3]; Tomasz Kowalczyk[3]; Piotr Zabielski[1]; [1]*Department of Medical Biology, Medical University of Bialystok, Bialystok, Poland;* [2]*1 st Clinical Department of General and Endocrine Surgery, Medical University of Białystok, Bialystok, Poland;* [3]*Clinical Research Center , Medical University of Białystok, Bialystok, Poland;* [4]*Department of Hygiene , Epidemiology and Metabolic Disorders , Medical University of Białystok, Bialystok, Poland*

MP 106   **A Novel, Q-ToF Data Independent Acquisition Method Using an RF Only Quadrupole with Scanning Dipolar Excitation**; <u>Keith Richardson</u>[1]; Martin Green[1]; Chris Hughes[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

MP 107   **Unequivocal structural analysis of a tryptic peptide despite isobaric interference using in-source CID and the SY technique**; <u>Dany Jeanne Dit Fouque</u>[1]; Alicia Maroto[1]; Rémy Lartia[2]; Antony Memboeuf[1]; [1]*CEMCA, Université de Brest, CNRS, Brest, France;* [2]*UMR CNRS 5250, ICMG FR-2607, Université Grenoble-Alpes, Grenoble, France*

DATA-DEPENDENT ACQUISITION
MP 108-112

MP 108   **Label-free single cell proteomics**; Hila Wolf-Levy[1]; Tom Fleischer[1]; Liran Shlush[1]; <u>Yishai Levin</u>[1]; [1]*Weizmann Institute of Science, Rehovot, Israel*

MP 110   **Boosting DDA acquisition rates via off-instrument 3-D feature detection**; Mathew Guiterrez[1, 2]; <u>Rob Smith</u>[1, 2]; [1]*Prime Labs, Inc., Missoula, MT;* [2]*University of Montana, Missoula, MT*

MP 111   **Adding an MS2-based filter prior to scoring to improve the speed of multiple modification searches in SpectroMine**; <u>Lynn Verbeke</u>[1]; Oliver M. Bernhardt[1]; Jan Muntel[1]; Lukas Reiter[1]; [1]*Biognosys AG, Schlieren, Switzerland*

MP 112   **Developments in Real-Time Search on an Orbitrap Tribrid mass spectrometer**; <u>Jesse D. Canterbury</u>[1]; Graeme Mcalister[1]; William D. Barshop[1]; Tony Zhao[1]; Aaron M Robitaille[1]; Romain Huguet[1]; [1]*Thermo Fisher Scientific, San Jose, California*

DATA-INDEPENDENT ACQUISITION
MP 113-136

MP 113   **Leveraging Infrared Multiphoton Dissociation for Selective Data Independent Acquisition**; <u>Joshua P Salem</u>[1]; Kristina Håkansson[1]; Nicholas Borotto[2]; [1]*University of Michigan, Ann Arbor, MI;* [2]*University of Nevada, Reno, NV*

MP 114   **Hybrid spectral library combining DIA-MS data and a targeted virtual library substantially deepens the proteome coverage**; <u>Ronghui Lou</u>[1]; Pan Tang[1]; Kang Ding[1]; Wenqing Shui[2]; [1]*ShanghaiTech University, Shanghai, China;* [2]*iHuman Institute, ShanghaiTech University, Shanghai, China*

MP 115   **High-precision ion mobility calibration greatly improves diaPASEF analysis**; <u>Tejas Gandhi</u>[1]; Stephanie Kaspar-Schoenefeld[2]; Oliver M. Bernhardt[1]; David Schlessinger[1]; Sven Brehmer[2]; Gary Kruppa[2]; Jan Muntel[1]; Lynn Verbeke[1]; Lukas Reiter[1]; [1]*Biognosys, Schlieren, Switzerland;* [2]*Bruker Daltonics, Bremen, Germany*

MP 116   **Using microflow LC-SWATH-MS with extensive peptide fractionation to interrogate the proteome of KRas-mutant cancer cells**; <u>César Alain Aguilar-Valdés</u>[1]; Juan F Martinez-Aguilar[2]; [1]*Escuela Nacional de Ciencias Biológicas, Instituto Politécnico Nacional, Miguel Hidalgo, Mexico;* [2]*Red de Apoyo a la Investigación-CIC-INCMNSZ, Universidad Nacional Autónoma de México, Coyoacán, Mexico*

MP 117   **A Data-independent Acquisition (DIA) Approach on Quadrupole Time-of-Flight Mass Spectrometry for In-depth Peptide Mapping of Monoclonal Antibody**; <u>Yonghai Lu</u>[1]; Zhaoqi Zhan[2]; [1]*Shimadzu (Asia Pacific) PTE LTD, Singapore, Singapore;* [2]*Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore*

MP 118   **Parallel accumulation – serial fragmentation combined with data-independent acquisition (diaPASEF): Bottom-up proteomics with near optimal ion usage**; Florian Meier[1]; <u>Stephanie Kaspar-Schoenefeld</u>[2]; Andreas-David Brunner[1]; Max Frank[3]; Annie Ha[3]; Isabell Bludau[1]; Eugenia Voytik[1]; Markus Lubeck[2]; Oliver Raether[4]; Ruedi Aebersold[5, 6]; Ben C. Collins[5]; Hannes L. Röst[3]; Matthias Mann[1, 7]; [1]*Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Bruker Daltonik, Bremen, Germany;* [3]*Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON;* [4]*Bruker Daltonik GmbH, Bremen, Germany;* [5]*Department of Biology, Institute of Molecular Systems Biology, ETH Zürich, Zurich, Switzerland;* [6]*Faculty of Science, University of Zürich, Zurich, Switzerland;* [7]*NFF Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

MP 119   **Deep Quantitative Phosphoproteomics by Data Independent Acquisition Mass Spectrometry**; Reta Birhanu Kitata[1]; Chia-Feng Tsai[2]; Wai-Kok Choong[3]; Pei-Yi Lin[1]; Yun-Chien Chang[1]; Bo-Shiun Chen[1]; Alexey I. Nesvizhskii[4]; Ting-Yi Sung[5]; <u>Yu-Ju Chen</u>[1, 6]; [1]*Institute of Chemistry, Academia Sinica, Taipei, Taiwan;* [2]*Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington;* [3]*Institute of Information Science, Academia Sinica, Taipei, Taiwan;* [4]*Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, Michigan;* [5]*Institute of Information Science, Academia Sinica, Taipei, Taiwan;* [6]*Department of Chemistry, National Taiwan University, Taipei, Taiwan*

MP 120   **Ion-networks: a generic data format capturing the full dimensionality of data (in)dependent acquisition mass spectrometry**; Sander Willems[1, 2]; Simon Daled[1, 2]; Bart Van Puyvelde[1, 2]; Laura De Clerck[1, 2]; Sofie Vande Casteele[1, 2]; Dieter Deforce[1, 2]; <u>Maarten Dhaenens</u>[1, 2]; [1]*Ghent University, Faculty of Pharmaceutical Sciences, Ghent, Belgium;* [2]*ProGenTomics, Ghent, Belgium*

MP 121   **Data dependent-independent acquisition (DDIA): fusion of bottom-up proteomics paradigms in a single LC-MS/MS experiment**; <u>Shenheng Guan</u>[1, 2]; Paul P. Taylor[3]; Ziwei Han[1]; Michael F. Moran[2, 4]; Bin Ma[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*Hospital for Sick Children, Toronto, Ontario;* [3]*Rapid Novor Inc, Waterloo, Ontario;* [4]*University of Toronto, Toronto, Ontario*

MP 122   **High throughput proteomics - Application of diaPASEF for short gradients**; Stephanie Kaspar-Schoenefeld[1]; Markus Lubeck[1]; <u>Scarlet Koch</u>[2]; Oliver Raether[1]; Gary Kruppa[2]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Bruker Daltonic GmbH, Bremen, Germany*

MP 123   **Mass Defect-based Carbonyl Activated Tags (mdCAT) for Multiplex Data-independent Acquisition Proteome Quantification**; <u>Siwen Zhang</u>[1]; Yi Di[2]; [1]*Shanghai Cancer Center and Institutes of Biomedical Sciences*

and §NHC Key Laboratory of Glycoconjugates Research, Fudan University,, shanghai, China; [2]Fudan University, Shanghai, China

MP 124   **The influence of tissue content on proteomic variation in high-grade serous ovarian cancer**; <u>Srikanth S Manda</u>[1]; Maiken M Espersen[2]; Rohan Shah[1]; Steven G Williams[1]; Natasha Lucas[1]; Dylan Xavier[1]; Sadia Mahboob[1]; Andrew Robinson[1]; Peter G Hains[1]; Brett Tully[1]; Roger R Redel[1]; Philip J Robinson[1]; Qing Zhong[1]; Anna Defazio[2]; Rosemary Balleine[1]; [1]*Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia;* [2]*Centre for Cancer Research, Westmead Institute for Medical Research, University of Sydney, Westmead, Australia*

MP 125   **Direct searching of DIA data catches up with sample-specific libraries**; Oliver M. Bernhardt[1]; Timothy Man[1]; Lucie Piecková[1]; Lynn Verbeke[1]; Maximilian J. Helf[1]; Tejas Gandhi[1]; Roland Bruderer[1]; <u>Lukas Reiter</u>[1]; [1]*Biognosys, Schlieren, Switzerland*

MP 126   **Optimization of DDA Library Size using Prior Search of DIA data Improves Analysis of Large DIA data sets**; <u>Weigang Ge</u>[1]; Wei Liu[1]; Rui Sun[1]; Nan Xiang[1]; Tiannan Guo[1]; [1]*Westlake University, Hangzhou, China*

MP 127   **High dynamic range proteome analysis with BoxCar DIA and super-resolution Orbitrap mass spectrometry**; Florian Meier[1]; <u>Kyle Fort</u>[2]; Arne Kreutzmann[2]; Daniel Marc Mourad[2]; Konstantin Aizikov[2]; Dmitry Grinfeld[2]; Johannes B Mueller[1]; André C Michaelis[1]; Alexander A. Makarov[2]; Matthias Mann[1, 3]; [1]*Max Planck Institute of Biochemistry, Planegg, Germany;* [2]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [3]*Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark*

MP 128   **Labeling-free monitoring of the mitochondrial proteome using peptide-centric DIA and diaPASEF methods**; <u>Brett S Phinney</u>[1]; Maxence Le Vasseur[1]; Michelle Salemi[1]; Jodi Nunnari[1]; [1]*UC Davis, Davis, CA*

MP 129   **Achieving true DIA analysis via 2DMS**; <u>Christopher Andrew Wootton</u>[1]; Tomos E. Morgan[1]; Bryan P. Marzullo[1]; Alina Theisen[1]; Anisha Haris[1]; Diana C. Palacio Lozano[1]; Yuko Pui Yiu Lam[1]; Mark P. Barrow[1]; Peter B O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom*

MP 130   **KDM1A Inhibition Enhances ESR2-mediated Tumor Suppression in Ovarian Cancer**; Prabhakar Pitta-Venkata[1]; Yihong Chen[1]; Bridgitte Palacios[1]; Ilanna Loeffel[1]; Sammy Pardo[1]; Dana Molleur[1]; Ratna Vadlamudi[1]; <u>Susan T. Weintraub</u>[1]; Gangadhara Sareddy[1]; [1]*University of Texas Health Science Center at San Antonio, San Antonio, TX 78229*

MP 131   **Single Shot FAIMS-DIA Optimization for Deep Coverage of the Proteome**; <u>Roland Bruderer</u>[1]; Oliver M. Bernhardt[1]; Lynn Verbeke[1]; Sega Ndiaye[2]; Claire Dauly[2]; Lukas Reiter[1]; [1]*Biognosys AG, Schlieren, Switzerland;* [2]*Thermo Fisher Scientific, Courtaboeuf, France*

MP 132   **A Globally-Accessible Supercomputer (Deepsearch) & New DIA protocol (eMRM) to Quantify Peptides and Differentiate Samples, Even Without a FASTA File**; <u>Gautam Saxena</u>[1]; Aleksandra Binek[2]; Simion Kreimer[2]; Aaron Robinson[2]; Jennifer E Van Eyk[2]; [1]*DeepDIA, Bethesda, MD;* [2]*Cedars-Sinai Medical Center, Los Angeles, CA*

MP 133   **Spectrum-centric searches augment existing spectral libraries for high quality sample-specific DIA libraries**; <u>Lilian Randolph Heil</u>[1]; William E. Fondrie[1]; Brian C. Searle[2]; William Stafford Noble[1]; Michael J. MacCoss[1]; [1]*University of Washington, Seattle, WA;* [2]*Institute for Systems Biology, Seattle, WA*

MP 134   **Data independent workflow using SWATH® acquisition for comprehensive cell culture media analysis**; Zuzana Demianova[1]; <u>Elliott Jones</u>[2]; David Cox[3]; Lei Xiong[2]; [1]*Sciex, Brea, CA;* [2]*SCIEX, Redwood Shores, CA;* [3]*SCIEX, Concord, ON*

MP 135   **InfineQ: Real-time cloud-based DIA data processing for high-throughput proteomics**; Artyom Pugachev[1]; <u>Arnoud Groen</u>[1]; [1]*ProteiQ Biosciences GmbH, Berlin, Germany*

MP 136   **Democratizing DIA analysis on public cloud infrastructures via Galaxy**; <u>Matthias Fahrner</u>[1]; Melanie Föll[1]; Björn Andreas Grüning[2]; Oliver Schilling[1]; [1]*Institute for Surgical Pathology, Faculty of Medicine, University of Freiburg, Freiburg, Germany;* [2]*Bioinformatics Group, Department of Computer Science, University of Freiburg, Freiburg, Germany*

DISEASE BIOMARKERS
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MP 137   **Establishing the Clinical Relevance of Glycoproteins in Pancreatic Cancer**; <u>Tiffany Thein</u>[1]; Abel Bermudez[1]; Jeremy Sharib[2]; Sarah M Totten[1]; Fernando Garcia-Marques[1]; Tyler York[2]; Keely Fuller[1]; Kimberly S Kirkwood[2]; Sharon J Pitteri[1]; [1]*Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA;* [2]*Department of Surgery, University of California San Francisco, San Francisco, CA*

MP 138   **Damaged vascular ECM proteins induced cardiovascular diseases by recruiting macrophages and LDLs to atherosclerotic plaque**; <u>Siu Kwan Sze</u>; *Nanyang Technological University, Singapore, Singapore*

MP 139   **Analysis of advanced glycation end products through LC-MS/MS for the early diagnosis of cancer**; Lakmini Senavirathna[1]; Ru Chen[2]; Sheng Pan[1]; [1]*University of Texas Health Science Center at Houston, Houston, TX;* [2]*Baylor College of Medicine, Houston, TX*

MP 141   **Novel Spatial N-Glycomic and Glycocalyx Profile of 3D Human Colon Cancer Cell Lines Utilizing a NanoLC-MS Base Platform**; Qing W Zhou[1]; Jennyfer Tena[1]; Carlito B Lebrilla[1]; [1]*University of California, Davis, Davis, CA*

MP 142   **Metabolic rewiring Modulates amyloid-like aggregates formation in Huntington's disease**; Sai Manohar Thota[1]; Sai Sanwid Pradhan[1]; Bhavana N Reddy[2]; Isha Verma[3]; Rajesh Babu D[4]; Vivek Tiwari[5]; Vidyasagar K[6]; Pavan Vasoya[6]; Ashish Pargaonkar[7]; Deepak Saligrama[7]; Sunil H V[8]; Krishna Murty V[9]; Seshagiri Polani[3]; Sanjaya Viswamitra[2]; Dileep Kumar[10]; Joshy E V[9]; Venketesh Sivaramakrishnan[1]; [1]*Department of Biosciences, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India;* [2]*Department of Radiology, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India;* [3]*Department of Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bengaluru, India;* [4]*Department of Chemistry, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India;* [5]*Centre for Brain Research, Indian Institute of Science, Bengaluru, India;* [6]*Department of Neurosurgery, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India;* [7]*Agilent Technologies, BENGALURU, India;* [8]*FDI + Care, Department of Nuclear Medicine and PET CT, Mazumdar Shaw Cancer Center, Bengaluru, India;* [9]*Department of Neurology, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India;* [10]*Siemens Healthcare Pvt Limited, Bengaluru, India*

MP 143   **Development of a high-content high-throughput screening platform using integrated omics to assess for impacts on metabolism**; John Janiszewski[1]; Matt Hall[1]; Sam Michael[1]; Richard Schneider[1]; Stephen Ferguson[2]; Michael Iannotti[1]; Rebecca Cardone[3]; Richard G. Kibbey[3]; Raghav Sehgal[3]; Qiushi Sun[3]; Surbhi Poddar[4]; Maheswari Karthikeyan[4]; Sunil Dhakad[4]; Darren Dumlao[5]; Elias Padilha[1]; Kelli Wilson[1]; [1]*NIH/NCATS, Rockville, MD;* [2]*NIH/NIEHS, Durham, NC;* [3]*Yale University, New Haven, CT;* [4]*Elucidata, Delhi, India;* [5]*SCIEX, Redwood Shores, California 1201*

MP 144   **Adenosine Deaminase reprograms metabolism and promotes onset and progression of Rheumatoid Arthritis (RA)**; Saikrishna Srimadh Bhagavatham[1]; Dr. Narsimulu Gumdal[2]; Dr. Narasimhan K[3]; Dr. Damodaram Potikuri[4]; Dr. Rajesh Babu Dandamudi[5]; Dr. Sai Mangala Divi[6]; Dr. Ashish Pargaonkar[7]; Dr. Rahul Ray[8]; Sujith Kumar Pulukool[1]; Dr. Vishnu Kannan[1]; Ashwin Ashok Naik[1]; Saibharath Simha Reddy Santha[1]; Dr. Prakash Khanchandani[8]; Dr. Venketesh Sivaramakrishnan[1]; [1]*Department of Biosciences, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India;* [2]*GVN Medical Centre, Hyderabad, India;* [3]*Sri Sathya Sai General Hospital, Puttaparthi, India;* [4]*Subodaya Rheumatology Centre, Tirupati, India;* [5]*Department of Chemistry, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India;* [6]*Department of Biochemistry, Sri Sathya Sai Institute of Higher Medical Sciences, Puttaparthi, India;* [7]*Agilent Technologies India Pvt Ltd, Bengaluru, India;* [8]*Department of Orthopedics, Sri Sathya Sai Institute of Higher Medical Sciences, Prasanthi Gram, Puttaparthi, India*

MP 145   **Breath Biopsy: combining Thermal Desorption-Gas Chromatography with High Resolution Mass Spectrometry for improved sensitivity and selectivity in untargeted breath analysis**; Dominic Roberts[1]; Lori Dolata[2]; Cristian Cojocariu[3]; Max Allsworth[4]; Jason Cole[5]; Paul Silcock[3]; [1]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [2]*Thermo Fisher Scientific, Austin, TX;* [3]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [4]*Owlstone Medical Ltd, Cambridge, United Kingdom;* [5]*Thermo Fisher Scientific, Austin, Texas*

MP 146   **Developing proteins and phosphoproteins in urine extracellular vesicles as biosignatures for Parkinson's disease diagnostics**; Marco Hadisurya[1]; Li Li[2]; Shalini Padmanabhan[3]; Anton Illiuk[4]; W. Andy Tao[1, 4]; [1]*Purdue University, West Lafayette, IN;* [2]*Tymora Analytical Operations, West Lafayette, IN;* [3]*The Michael J. Fox Foundation, New York City, NY;* [4]*Tymora Analytical, West Lafayette, IN*

MP 147   **Robust Plasma Protein Profiling Workflow for Routine Clinical Research Using a UHPLC and a Modified Orbitrap Mass Spectrometer**; David Sarracino[1]; Christian Klaas[2]; Bradley J Hart[3]; Shen Luan[1]; Amol Prakash[4]; Xiaolei Xie[5]; Debadeep Bhattacharyya[1]; [1]*Thermo Fisher Scientific, Cambridge, MA;* [2]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [3]*ThermoFisher Scientific, San Jose, CA;* [4]*Optys Tech Corporation, Shrewsbury, MA;* [5]*Thermo Fisher Scientific, San Jose, California*

MP 148   **Mass spectrometry-based proteomics of liquid biopsies for neurodegenerative diseases screening**; Svitlana Rozanova[1]; Katalin Barkovits[1]; Katrin Marcus[1]; [1]*Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany*

MP 149   **Top-down LC/MS Analysis of Cardiac Troponin I Proteoforms from Clinical Blood Samples of Acute Myocardial Infarction**; Timothy Tiambeng[1]; David S Roberts[1]; William H. Swain[2]; Daniel Kim[1]; Song Jin[1]; Ying Ge[1, 3, 4]; [1]*Chemistry Department University of Wisconsin-Madison, Madison, WI 53705;* [2]*University of Wisconsin School of Medicine and Public Health, Madison, WI;* [3]*Human Proteomics Program, School of Medicine and Public Health, Madison, WI;* [4]*Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI*

MP 150   **Identification of Biomarkers for Glioblastoma in Saliva using UPLC-IM-MS**; Amy N. W. Schnelle[1]; Christina A. Gaw[1]; Luke T. Richardson[1]; Fengfei Wang[2]; Erxi Wu[2]; Touradj Solouki[1]; [1]*Baylor University, Waco, TX;* [2]*Neuroscience Institute and Department of Neurosurgery, Baylor Scott & White Health, Temple, TX*

MP 151   **Proteomic Profiling of Extracellular Vesicles Isolated from Human Alzheimer's Disease Brain Tissues**; Manveen K Sethi[1]; Satoshi Muraoka[1]; Annina M. Deleo[1]; John D. Hogan[1]; Tsuneya Ikezu[1]; <u>Joseph Zaia</u>[1]; [1]*Boston University School of Medicine, Boston, MA*

MP 152   **Protein Signatures to Distinguish Aggressive from Indolent Prostate Cancer**; <u>Fernando Garcia-Marques</u>[1]; Shiqin Liu[1]; Sarah M Totten[1]; Abel Bermudez[1]; Rosalie Nolley[2]; Cheylene Tanimoto[1]; En-Chi Hsu[1]; Tanya Stoyanova[1]; James D. Brooks[1, 2]; Sharon J Pitteri[1]; [1]*Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA;* [2]*Department of Urology, Stanford University School of Medicine, Stanford, CA*

MP 153   **Proteomic Profiling of Small Extracellular Vesicles Secreted by Human Pancreatic Cancer Cells Implicated in Cellular Transformation**; <u>Kelly Servage</u>[1]; Karoliina Stefanius[1]; Kim Orth[1]; [1]*UT Southwestern Medical Center, Dallas, TX*

MP 154   **EPHX2 downregulation in the arachidonic acid pathway is associated with poor clinical outcomes in male bladder cancer patients**; Roshan Borkar[1]; <u>Shiva Shankar Ravi</u>[1]; Danthasinghe Waduge Badrajee Piyarathna[1]; Karthik Reddy Kami Reddy[1]; Dimuthu Perera[1]; Martha K Terris[2]; Kimiko L Krieger[1]; Roni J Bollag[2]; Stephen B Williams[3]; Kimal Rajapakshe[1]; Leomar Y Ballester[4]; Balasubramanyam Karanam[5]; Shyam M. Kavuri[1]; Minjae Lee[6]; Arun Sreekumar[1]; Yair Lotan[7]; Cristian Coarfa[1]; Nagireddy Putluri[1]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Augusta Universuty, Augusta, GA;* [3]*University of Texas Medical Branch at Galveston, Galveston, TX;* [4]*University of Texas at Houston Health Science Center, Houston, Texas;* [5]*Tuskegee University, Tuskegee, AL;* [6]*University of Texas Health Science Center at Houston, Houston, TX;* [7]*UT Southwestern Medical Center, Dallas, TX*

MP 157   **Proteomics Studies in Parkinson's Disease**; <u>George S. Katselis</u>[1]; Paulos Chumala[1]; Brooke Thompson[1]; Savannah Eanes[1]; Sarah Bocking[1]; Alex Rajput[1]; Ali Rajput[1]; [1]*University of Saskatchewan, Saskatoon, SK*

MP 158   **Redox regulation of glutathione per/polysulfide in hyperglycemic endothelial cells**; <u>Xinggui Shen</u>[1]; Christopher G. Kevil[1]; [1]*Department of Pathology, LSU Health-Shreveport, Shreveport, Louisiana*

MP 160   **Direct, MALDI-ToF mass spectrometry, detection of SARS-1 and SARS-2 (COVID-19) fusion glyco-peptide ejected from Spike proteins**; Jason Iles[1]; <u>Ray Iles</u>[2]; George Carnell[1]; Raminta Zmuidinaite[2]; Alexander Sampson[1]; Matteo Ferrari[3]; Angalee Nadesalingam[1]; Sneha Vishwanath[1]; Jonathan Heeney[1]; [1]*University of Cambridge, Cambridge, United Kingdom;* [2]*MAP Sciences, Bedford, United Kingdom;* [3]*DIOSynVax, Cambridge, United Kingdom*

MP 161   **Discovery proteomics for the detection of diagnostic markers in an experimental model of equine septic arthritis using LC-MS/MS**; <u>Roman V. Koziy</u>[1]; Paulos Chumala[2]; Elemir Simko[1]; Georgios S. Katselis[2]; [1]*Department of Pathology, Western College of Veterinary Medicine, University of Saskatchewan, Saskatoon, SK;* [2]*Department of Medicine, Canadian Centre for Health and Safety in Agriculture, College of Medicine, University of Saskatchewan, Saskatoon, SK*

MP 162   **Aberrant N-glycosylation patterns related to serum IgG subclasses in Idiopathic membranous nephropathy**; <u>Clizia Chinello</u>[1]; Noortje De Haan[2]; Giulia Capitoli[3]; Barbara Trezzi[4]; Antonella Radice[5]; Stefania Galimberti[3]; Manfred Wuhrer[2]; Renato Alberto Sinico[4]; Fulvio Magni[6]; [1]*Clinical Proteomics & Metabolomics Unit, Dep. of Medicine and Surgery, UNIMIB, Vedano al Lambro, Italy;* [2]*Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands;* [3]*Centre of Biostatistics for Clinical Epidemiology, Dep. of Medicine and Surgery, UNIMIB, Monza, Italy;* [4]*Nephrology Unit, Dep. of Medicine and Surgery, UNIMIB, Monza, Italy;* [5]*Microbiology and Virology Department, San Carlo Borromeo Hospital, Milan, Italy;* [6]*Clinical Proteomics & Metabolomics Unit, UNIMIB, Dep. of Medicine and Surgery, Vedano al Lambro, Italy*

DRUG DISCOVERY/DMPK/ADME I
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MP 163   **A novel G protein-biased and subtype selective agonist for a G protein-coupled receptor discovered from screening herbal extracts**; Bingjie Zhang[1]; Simeng Zhao[1]; Ye Xin[1]; <u>Wenqing Shui</u>[1]; [1]*iHuman Institute, ShanghaiTech University, Shanghai, China*

MP 164   **An LC-MS/MS assay for quantification of Evans Blue to aid in blood content correction during tumor penetration assessment of nanomedicines**; <u>Nicole Bebrin</u>[1]; Linlin Dong[1]; Kojo Abdul-Hadi[1]; Robert Griffin[1]; Dong Wei[1]; Mark G Qian[1]; [1]*Takeda Pharmaceuticals International Co., Cambridge, MA*

MP 165   **Mass Spectrometer Data Quality at High-Acquisition Rate for In-Vitro Assays Matrices Analyzed in Less than 1 Second per Sample**; <u>Jean Lacoursière</u>[1]; Serge Auger[1]; Francis Brière[2]; Pier-Luc Plante[2]; Pierre Picard[1]; [1]*Phytronix Technologies, Quebec, QC;* [2]*Université Laval, Quebec, Quebec*

MP 166   **Ultra High-Throughput and Chromatography-Free Bioanalysis of Polar Analytes with Acoustic Ejection Mass Spectrometry**; Andrew Wagner[1]; Jun Zhang[1]; Chang Liu[2]; Tom Covey[2]; Timothy Olah[1]; Harold Weller[1]; <u>Wilson Shou</u>[1]; [1]*Bristol-Myers Squibb, Princeton, NJ;* [2]*SCIEX, Concord, ON*

MP 167   **Assaying Protein / Ligand Binding with High-Resolution Native Mass Spectrometry**; Matthias Witt[1]; Christopher Thompson[2]; Yongwei (peter) Wang[3]; Michael Greig[4]; <u>Marshall W. Bern</u>[5]; Xuefei Yin[5]; Ilker Sen[5]; Jia Liu[6]; Yang Ye[6]; [1]*Bruker Daltonic GmbH, Bremen, Germany;* [2]*Bruker Scientific LLC, Billerica, MA;* [3]*Bruker*

Daltonics, shanghai, China; [4]Bruker Scientific, San Jose, CA; [5]Protein Metrics, Cupertino, CA; [6]Shanghai Institute of Materia Medica, Pudong, China

MP 168 **Direct determination of total, encapsulated and free doxorubicin concentrations in human plasma to support bioequivalence studies of liposomal doxorubicin**; Yuhuan Ji[1]; Xueyuan Zhang[2]; Jinzhi Liu[1]; Yu Chen[1]; Ji Liu[1]; Chunlei Li[2]; Min Meng[1]; <u>Laixin Wang</u>[1]; *[1]Chongqing Denali Medpharma Co.,Ltd, Chongqing, China; [2]CSPC Pharmaceutical Group Ltd, Shijiazhuang, China*

MP 169 **Measurement of Free Concentrations of Testosterone Using Newly Developed SpinTip Microextraction Devices with Polyacrylonitrile**; <u>Daniel Galke</u>[1]; F. Marcel Musteata[1]; *[1]Albany College of Pharmacy and Health Sciences, Albany, NY*

MP 170 **LC-MS/MS quantification of Withaferin A and 12-Deoxywithastramonolide in mouse plasma and brain following oral administration of ashwagandha herbal extract solution**; Ludmila Alexandrova[1]; <u>Zijie Xia</u>[1]; Edwin Chang[2]; Chirag B. Patel[2, 3]; Corinne Beinat[2]; Luis Avila[4]; Lal Hingorani[5]; Sanjiv S. Gambhir[2, 6, 7]; Allis S. Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford University, Stanford, CA; [2]Department of Radiology, Molecular Imaging Program at Stanford (MIPS), Stanford University School of Medicine, Stanford, CA; [3]Department of Neurology and Neurological Sciences, Stanford University School of Medicine, Stanford, CA; [4]Aveta Biomics, Bedford, MA; [5]Pharmanza Herbal Pvt Ltd., Kansari, India; [6]Department of Bioengineering, Stanford University, Stanford, CA; [7]Department of Materials Science and Engineering, Stanford University, Stanford, CA*

MP 171 **A Multi-Channel LC/MS/MS platform for High-Throughput Bioanalysis in Drug Discovery**; <u>Hong Tsao</u>[1]; Scott Carrier[1]; Joseph Janiszewski[2]; Wayne Lootsma[2]; Steve Ainley[2]; *[1]Vertex Pharmaceuticals, Boston, MA; [2]Sound Analytics, Niantic, CT*

MP 172 **Proteolytic activity of enzyme beta lytic metalloendopeptidase as a potential antibacterial agent**; <u>Mihail Konstantinov</u>[1, 2]; Alexey Afoshin[3]; Irina Kudryakova[3]; Natalia Vasilyeva[3]; Ilya Toropygin[4]; *[1]Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; [2]Pirogov Russian National Research Medical University, Moscow, Russia; [3]G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Pushchino, Russia; [4]Orekhovich Institute of Biomedical Chemistry, Moscow, Russian Federation*

MP 173 **QTAP analysis of transporters for validation of human brain microvascular endothelial cell line as anin vitrohuman BBB model**; <u>Mouhssin Oufir</u>[1]; Jordan Goncalves[1]; Gregoire Harichaux[1]; Yann Courbebaisse[2]; Isabell Seibert[3]; Henriette Meyer Zu Schwabedissen[3]; Fabrice Viviani[1]; Matthias Hamburger[3]; *[1]Oncodesign, Villebon-Sur-Yvette, France; [2]ADOCIA, LYON, France; [3]UNIVERSITY OF BASEL, BASEL, Switzerland*

MP 174 **The novel data-mining strategy for metabolite identification based onUHPLC-Q-Exactive hybrid quadrupole orbitrapHRMS: Application to Prucalopride**; Lihua Zuo[1]; Liwei Liu[2]; Yingying Shi[2]; Zhuolun Li[2]; Xiaojian Zhang[2]; <u>Zhi Sun</u>[2]; *[1]The First Affiliated Hospital of Zhengzhou University, Zhengzhou, China; [2]The First Affiliated Hospital of Zhengzhou University, Zhengzhou, China*

ELEMENTAL ANALYSIS: ICP/MS
MP 175-179

MP 175 **Pyrrole-based Conductive Polymer for Dispersive Solid-Phase Extraction and Quantification of Rare Earths Elements from Aqueous Media using ICP-MS**; <u>Govind Sharma Shyam Sunder</u>; *The University of Toledo, Toledo, OH*

MP 176 **UsingICP-MS/MS with M-Lens for the analysis of high silicon matrix samples**; <u>Yu Ying</u>[1]; Xiangcheng Zeng[1]; *[1]Agilent Technologies, China, Shanghai, China*

MP 177 **High Accuracy Quantification of Magnesium and Other Ionic Elements in Mice Through the Use of Isotope Dilution Mass Spectrometry (IDMS)**; <u>Ashley Parisi-Goldblatt</u>[1]; James Henderson[2]; Evan Ray[3]; Howard M. Kingston[2]; *[1]Duquesne University, Pittsburgh, PA; [2]Duquesne University, Pittsburgh; [3]University of Pittsburgh, Pittsburgh, PA*

MP 178 **An Innovative Platform Merging Elemental (LA-ICP-MS) and Biochemical (FTIR Imaging) Analysis for Biological Tissues**; <u>Khalid A. Al-Saad</u>[1]; Fazle Rakib[1]; Mohamed Ali[2]; Rafif Al-Saady[3]; Erik Goormaghtigh[4]; *[1]Qatar University, Doha, Qatar; [2]Qatar Biomedical Research Institute, Doha, Qatar; [3]Al Ahli Hospital, Doha, Qatar; [4]Université Libre de Bruxelles, Brussels, Belgium*

MP 179 **Simultaneous Determination of Heavy Metal and Mineral Content in Fruit Juices by Inductively Coupled Plasma Mass Spectrometry** ; <u>Raymond Li</u>[1]; Regina Tan[2]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [2]National University of Singapore, Singapore, Singapore*

ELEMENTAL ANALYSIS: ISOTOPE RATIO MS
MP 180-182

MP 180   **Cryofocus fast gas chromatography combustion isotope ratio mass spectrometry featuring a low temperature catalytic combustion reactor**; Rj Scott Lacombe[1]; Andrew Jones[2]; J. Thomas Brenna[1]; Herbert J Tobias[1]; *[1]Dell Pediatric Research Institute, University of Texas at Austin, Austin, TX; [2]Activated Research Company, Eden Prairie, MN*

MP 181   **Advanced Data Acquisition and Processing for the Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD)/Orbitrap Q Exactive Coupling for Improved Elemental/Isotopic Analysis**; Jacob R Bills[1]; Konstantin O. Nagornov[2]; Anton N. Kozhinov[2]; Yury O. Tsybin[2]; Tyler J. Williams[1]; R. Kenneth Marcus[1]; *[1]Clemson University, Clemson, SC; [2]Spectroswiss, Lausanne, Switzerland*

MP 182   **Determination of uranium isotope ratio in nuclear material samples using Thermal Ionization Mass Spectrometry**; Jung Youn Choi[1]; Youn-Joong Jeong[2]; Hana Seo[1]; Haneol Lee[1]; Tae Hee Kim[1]; Chan Jong Park[1]; Hyun Young Kim[1]; *[1]Korea Institute of Nuclear Nonproliferation and Control, Daejeon, South Korea; [2]Korea Basic Science Institute, Ochang, Cheongju-si, South Korea*

ELEMENTAL ANALYSIS: SIMS AND SURFACE ANALYSIS
MP 183-186

MP 183   **Detecting trace level biosignatures in fossils using cluster beam Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS)**; Naoko Sano[1]; Allen Bellew[1]; Graham W.H. Purvis[2]; Paul Blenkinsopp[1]; *[1]Ionoptika Ltd, Eastleigh, United Kingdom; [2]Earth, Ocean & Planetary Science Research, School of Natural and Environmental Sciences, Newcastle University, Newcastle upon Tyne, United Kingdom*

MP 184   **Micro- and Nanoscale Understanding of Phosphorus-Based Antiwear Films on Steel Surfaces**; Matthias Lorenz[1, 2]; Alison A. Pawlicki[1, 2]; Kerry Cogen[3]; Hitesh Thaker[3]; Olga S. Ovchinnikova[2]; *[1]University of Tennessee Knoxville, Knoxville, Tennessee; [2]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; [3]Infineum USA L.P., Linden, NJ*

MP 185   **Time-resolved time-of-flight secondary ion mass spectrometry for in-situ characterization of functional materials**; Anton Ievlev[1]; Olga S. Ovchinnikova[2]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN*

MP 186   **Resonance Ionization Mass Spectrometry for trace analysis of solids: depth profiling with flat-top laser ablation probe**; Igor V. Veryovkin[1]; C. Emil Tripa[1]; Jason M. Gross[1]; Luke Hanley[1]; Amy J. G. Jurewicz[2]; Donald S. Burnett[3]; *[1]University of Illinois at Chicago (UIC), Chicago, IL; [2]Arizona State University, Tempe, AZ 85287; [3]California Institute of Technology, Pasadena, CA*

FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS I
MP 187-207

MP 187   **SPME Arrow-a novel solid-phase microextraction device for determination of PAHs in drinking water by gas chromatography tandem Mass spectrometry**; Xiaolei Shi; *Shimadzu (China) Co., Ltd., Shanghai Office, Shanghai, China*

MP 188   **Towards development of a matrix-independent calibration strategy for targeted quantification of milk allergens**; Bini Ramachandran[1]; Charles Yang[2]; Melanie Downs[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, California*

MP 189   **Multi-class Veterinary Drug Screening and Quantitation by High Resolution Mass Spectrometry (HRMS) using a Modified Quadrupole-Orbitrap Mass Spectrometer**; Ed George[1]; Laura Burns[2]; Dwayne Schrunk[3]; Viet Dang[4]; Charles Yang[5]; Dipankar Ghosh[4]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Iowa State University, Ames, IA; [3]Iowa State Univ College of Veterinary Medicine, Ames, IA; [4]Thermo Fisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific, San Jose, California*

MP 190   **Rapid MALDI-TOF-based Proteomics approach for fast and reliable detection of Feta cheese adulteration**; Anastasia S. Kritikou[1]; Dimitrios E Damalas[1]; Ioanna V. Barla[1]; Reza Aalizadeh[1]; Volker Sauerland[2]; Bob Galvin[2]; Carsten Baessmann[2]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Athens, Greece; [2]Bruker Daltonik GmbH, Bremen, Germany*

MP 191   **Quantitative Analysis of Blended Oils by Matrix-assisted Laser Desorption/Ionization Mass Spectrometry and Partial Least Squares Regression**; Suying Li[1]; Tsz-Tsun Ng[1]; Zhong-Ping Yao[1]; *[1]The Hong Kong Polytechnic University, Hung Hom, Hong Kong*

MP 192   **Metabolomics profiling for identification of the bioactive constituents in Taiwan aboriginal herb using high-resolution mass spectrometry**; Hong-jhang Chen[1]; GUI-RU Xie[1]; *[1]National Taiwan University, Taipei, Taiwan*

MP 193   **Evaluating the quantification of soy protein in incurred matrices using a targeted LC-MS/MS method**; Jenna Krager[1]; Joseph L. Baumert[1]; Melanie L. Downs[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE*

MP 194   **Targeted Peptide Quantitation of Seven Food Allergens in Dark Chocolate Using Triple Quadrupole LC/MS**; Lee Sun New[1]; Jerry Zweigenbaum[2]; Chee Sian Gan[1]; [1]*Agilent Technologies Singapore (Sales) Pte Ltd, Singapore, Singapore;* [2]*Agilent Technologies, Wilmington, DE*

MP 195   **Quantitation of Patulin in Apple Juice and Apple Products using a compact mass spectrometer**; Daniel Eikel[1]; Changtong Hao[1]; Simon Prosser[1]; [1]*Advion Inc., Ithaca, NY*

MP 196   **Peanut Allergens Survive Excessive Dry Thermal Processing**; Lee K Palmer[1]; Justin T Marsh[1]; Joseph L Baumert[1]; Philip E Johnson[1]; [1]*University of Nebraska-Lincoln, Lincoln, NE*

MP 197   **Structure elucidation of ultra-trace monoenes in milk and polymethylene-interrupted PUFA with fragmentation rules by solvent-mediated covalent adduct chemical ionization MS/MS**; Donghao Wang[1]; Zhen Wang[1]; J. Thomas Brenna[1]; [1]*University of Texas at Austin, Austin, Texas*

MP 198   **Developing an integrated high-throughput spectroscopic strategy for better understanding of food metabolomics**; Ruey Leng Loo[1, 2]; Samantha Lodge[1, 3]; Berin Boughton[1]; Melvin C.L. Gay[4]; Heino M. Heyman[5]; Christopher Thompson[5]; Elaine Holmes[1, 2]; Jeremy Nicholson[1, 3]; [1]*Australian National Phenome Centre, Murdoch University, Murdoch, Australia;* [2]*Research and Innovation Office, Murdoch University, Murdoch, Australia;* [3]*Health Futures Institute, Murdoch University, Murdoch, Australia;* [4]*Bruker Pty Ltd, Victoria, Australia;* [5]*Bruker Daltonics, Billerica, MA*

MP 199   **Development of a real time direct-MS screening technique for commonly encountered adulteration and contamination scenarios in edible oils**; Sara Stead[1]; Nicola Dreolin[1]; Pierre-Alain Golay[2]; Francesca Giuffrida[2]; Kornel Nagy[2]; Lindsay Hatch[3]; Kenneth Rosnack[4]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Societe des Produits Nestle S.A., Lausanne, Switzerland;* [3]*Waters Corporation, Beverly, MA;* [4]*Waters Corporation, Milford, MA*

MP 200   **Classification of Bacterial Strains with the Multi-ionization Platform and Open Mass Fingerprinting Framework (OMFF)**; Abigail Moreno-Pedraza[1, 2]; Darrell D. Marshall[3, 4]; Sandra Martínez-Jarquín[2]; Santosh Karki[1, 3]; Khoa Hoang[3]; Milan Pophristic[3]; Vladimir Shulaev[5]; Charles N. Mcewen[3, 6]; Robert Winkler[2]; Sarah Trimpin[1, 3]; [1]*Department of Chemistry, Wayne State University, Detroit, Michigan;* [2]*Department of Biochemistry & Biotechnology, CINVESTAV, Irapuato, Mexico;* [3]*MSTM, LLC, Newark, Delaware;* [4]*Total Analysis LLC, Detroit, Michigan;* [5]*University of North Texas, Denton, TX;* [6]*Department of Chemistry & Biochemistry, University of the Sciences, Philadelphia, PA*

MP 201   **Workflow for food classification and authenticity using yerba mate and high-resolution GC/Q-TOF**; Sofia Nieto[1]; Melissa Churley[1]; [1]*Agilent Technologies, Inc., Santa Clara, CA*

MP 202   **Post-harvest storage influences volatile aroma profiles of melon varieties identified by HS-SPME-GC-MS**; Varsha Ravi[1]; Jashbir Singh[2]; Rita Metrani[2]; G. K. Jayaprakasha[2]; Bhimanagouda S. Patil[2]; [1]*Texas A&M university, College station, TX;* [2]*Texas A&M University, College Station, TX*

MP 203   **Widely targeted metabolomics of hydrophilic compounds using LC-MS/MS -How compounds change when curry is stored overnight?-**; Takanari Hattori[1]; Harumi Kubo[1]; Yasuko Yamada[2]; Jun Watanabe[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Shimadzu Techno-Research, Inc., Kyoto, Japan*

MP 204   **Nontargeted and Statistical Approaches for Honey Authenticity Analysis**; Katherine Hyland[1]; Diana Tran[2]; [1]*SCIEX, Redwood City, CA;* [2]*SCIEX, Redwood Shores, California 1201*

MP 205   **Highly sensitive analysis of the related substance of ciguatoxins by the multiple reaction monitoring and electrospray ionization with LC/MS/MS**; Manami Kobayashi[1]; Kota Ishioka[1]; Junichi Masuda[1]; Yoshihiro Hayakawa[2]; [1]*Shimadzu Corporation, Hadano, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan*

MP 206   **Optimization of a targeted, multi-allergen LC-MS/MS method for the quantification of egg, milk, and peanut in food**; Weili Xiong[1]; Christine H. Parker[1]; Katherine L. Fiedler[1]; [1]*U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, College Park, MD*

MP 207   **Authentication of Vegetable Oils: Determination of Glyceride and Free Fatty Acid by Liquid Chromatography-High Resolution Mass Spectrometry**; Lihai Guo[1]; Lijun Li[1]; Nick Zhu[1]; Rui Gong[2]; Zong Yang[1]; [1]*SCIEX, Shanghai, China;* [2]*Wuhan Institute for Food and Cosmetic Control, Wuhan, China*

FUNDAMENTALS: PHOTODISSOCIATION
MP 208-214

MP 208   **Wavelength-Tunable Ultraviolet Photodissociation for Structural Analysis of Unsaturated Lipids**; Hai-Fang Li[1]; Jing Zhao[2]; Wenbo Cao[1]; Yu Xia[2]; Zheng Ouyang[1]; [1]*Department of Precision Instrument, Tsinghua University, Beijing, China;* [2]*Department of Chemistry, Tsinghua University, Beijing, China*

MP 209   **Differentiation of Peptide Isomers by Modulated Excited-State Dissociation**; Brielle L. Van Orman[1]; Hoi-Ting Wu[1]; Ryan R. Julian[1]; [1]*University of California, Riverside, Riverside, CA*

MP 210   **Probing Proline Cis/Trans Isomer Scrambling During ESI With Radical-Directed Dissociation**; Jacob W Silzel[1]; Miklos Guttman[2]; Ryan R. Julian[3]; [1]*UC Riverside, Riverside, CA;* [2]*University of Washington, Seattle, WA;* [3]*University of California, Riverside, Riverside, CA*

MP 211   **Influence of the aromatic moiety on gas phase reactions of heptamethine cyanine dyes using femtosecond-laser-pulse induced photodissociation**; Elena Mitrofanov; Tassilo Muskat; Jurgen Grotemeyer; *Christian-Albrechts-Univ, Kiel, Germany*

MP 212   **Specific detection of cysteine sulfenic acid by coupling mass spectrometry with Laser Induced Dissociation**; Jean-Valéry Guillaubez[1]; Delphine Pitrat[2]; Yann Bretonnière[2]; Jérôme Lemoine[1]; Marion Girod[1]; *[1]University of Lyon, Villeurbanne, France; [2]ENS Lyon, Lyon, France*

MP 213   **Characterization of Transglutaminase-Directed Chromophore-Tagged Proteins by Ultraviolet Photodissociation**; Amanda Helms[1]; Amissi Sadiki[2]; Zhaohui Sunny Zhou[2]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Northeastern University, Boston, MA*

MP 214   **UVPD Fragmentation of Intact Proteins: Comparison of 193 nm versus 213 nm photoactivation**; Michael B Lanzillotti[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, Texas*

GLYCOPROTEINS I
MP 215-234

MP 215   **Enhancing Glycopeptide Detection, Identification, and Structural Characterization through PGC-Incorporated LC-IMS**; Daniel Delafield[1]; Lingjun Li[2]; *[1]University of WIsconsin, Madison, WI; [2]University of Wisconsin, Madison, WI*

MP 216   **A workfolw for the Large Scale Quantitative Proteomics and N-Glycoproteomics Analysis of Cancer Cells**; Xiaoxu Tian[1]; Ping Wu[1]; Chen Su[1]; Yue Yin[1]; Chao Peng[1]; *[1]National Facility for Protein Science, Zhangjiang Lab,SARI, CAS, Shanghai, 201210, China, shanghai, China*

MP 218   **Developing a new pipeline for mapping and quantification of O-glycosylation using isobaric N, N-dimethyl leucine (DiLeu) reagents**; Qinying Yu[1]; Zhengwei Chen[1]; Xiaofang Zhong[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 219   **Simple and fast assay for apolipoprotein E phenotyping and glycotyping: Discovering isoform-specific glycosylation in plasma and cerebrospinal fluid (CSF)**; Yueming Hu[1]; Hussein N Yassine[2]; Dobrin Nedelkov[1]; *[1]Isoformix Inc., Phoenix; [2]University of Southern California, Los Angeles, CA*

MP 220   **Efficient MS-based workflows for analysis of released glycans, glycopeptides, and glycosylated intact proteins in biopharmaceutical development**; Catherine Evans[1]; Jonathan Jones[2]; Peter Haberl[3]; Maurizio Bronzetti[4]; *[1]Genedata AG, Basel, Switzerland; [2]Genedata Ltd, Cambridge, United Kingdom; [3]Genedata GmbH, Munich, Germany; [4]Genedata Inc, San Francisco, CA*

MP 221   **Quantitative proteomics reveals distinct distribution and degradation patterns of O-GlcNAcylated proteins in the nucleus and the cytoplasm**; Senhan Xu[1]; Ming Tong[1]; Suttipong Suttapitugsakul[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 222   **MS/MS Filtering and Wildcard Searches for Novel N- and O-linked Glycopeptide Identifications**; K. Ilker Sen[1]; Shruti Nayak[2]; Beatrix Ueberheide[2]; Yong J Kil[3]; Doron Kletter[3]; Marshall W. Bern[3]; *[1]Protein Metrics Inc., Cupertino, CA; [2]New York University School of Medicine, New York, NY; [3]Protein Metrics Inc, Cupertino, CA*

MP 223   **Comprehensive Analysis of IgE Glycoforms by FAIMS-LC-MS/MS using Orbitrap Eclipse Mass Spectrometer**; Aman Makaju[1]; Kim Alving[2]; Bing Wang[2]; Rosa Viner[1]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Sanofi, Waltham, MA*

MP 224   **UPLC-MS Assessment on the Structural Similarity of Recombinant Human Erythropoietin (rhEPO) Analogues from Manufacturers in China for Attribute Monitoring**; Henry Shion[1]; Lei Tao[2]; William Alley[1, 3]; Chunming Yao[2]; Ying Qing Yu[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, Massachusetts; [2]National Institute for Food and Drug Control, Beijing, China; [3]Texas A&M University - San Antonio, San Antonio, TX*

MP 225   **N-Linked Glycoproteome Analysis of Bovine Milk Exosomes**; Xuyao Zeng[1]; Brooke A. Brown[1]; Kathleen T. Grassmyer[1]; Jonathan C. Trinidad[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

MP 226   **High-sensitivity N-glycan profiling of human plasma and blood-derived immunoglobulin G and extracellular vesicle isolates using capillary zone electrophoresis-mass spectrometry**; Anne-Lise Marie[1]; Somak Ray[1]; Shulin Lu[2]; Jennifer Jones[3]; Ionita Ghiran[2]; Alexander R. Ivanov[1]; *[1]Barnett Inst., Northeastern University, Boston, MA; [2]Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA; [3]NIH/NCI/CCR, Bethesda, MD*

MP 227   **Glycomic and Glycoproteomic Analysis of Brain N-Glycosylation in High Fat Diet-Induced Obese Mice**; Mackenzie Honeycutt[1]; Jennyfer Tena[1]; Miranda Krueger[1]; Helen Raybould[1]; Carlito B Lebrilla[1]; Mariana Barboza[1]; *[1]University of California Davis, Davis*

MP 228   **G-FORGE: Novel Machine Learning Software for Automated Large Scale Intact Glycoproteomics Profiling in A Multidimensional Separation (CE/IEF/HILIC + LCMS) Workflow**; Jiana Duan[1]; Erika Cline[1]; Shengkun Dai[1]; Steven Patrie[1]; *[1]Northwestern University, Evanston, IL*

MP 229   **Metabolic Engineering Challenges to extending N-glycan pathways in CHO cells**; Qiong Wang[1]; Tiexin Wang[2]; Shuang Yang[3]; John Cipollo[3]; Michael J. Betenbaugh[1]; [1]*JHU Chemical Engineering Department, Baltimore;* [2]*JHU Chemical Engineering Department, Baltimore, Maryland;* [3]*FDA Laboratory for Bacterial Polysaccharides, Silver Spring, Maryland*

MP 230   **Combining Depletion and Fractionation for Deep Site-Specific Profiling of the Urinary Glycoproteome**; John Froehlich[1]; Shannon E. DiMartino[2]; [1]*Boston Childrens Hospital, Boston, MA;* [2]*Boston Children's Hospital, Boston*

MP 231   **An O-GlcNAc modified protein promotes seed germination and flowering by modulating alternative RNA splicing and transcription of key regulators**; Shouling Xu; *Carnegie Institution at Stanford, Stanford, CA*

MP 232   **Low collision energy fragmentation in the structure-specific glycoproteomics analysis**; Miloslav Sanda[1]; Julius Benicky[1]; Zuzana Brnakova Kennedy[1]; Radoslav Goldman[1]; [1]*Georgetown University, Lombardi Cancer Center, Washington, DC*

MP 233   **Glycosylation at an evolutionary nexus: both vertebrate and invertebrate N-glycomic features are expressed by the brittle star Ophiactis savignyi**; Barbara Eckmair[1]; Chunsheng Jin[2]; Daniel Abed-Navandi[3]; Iain B. H. Wilson[1]; Katharina Paschinger[1]; [1]*University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria;* [2]*Goteborgs universitet, Goteborg, Sweden;* [3]*Haus des Meeres - Aqua Terra Zoo, Vienna, Austria*

MP 234   **New insights into the honeybee N-glycome byoff-line LC-MS analysis**; Alba Hykollari[1]; Daniel Malzl[2]; Jorick Vanbeselaere[2]; Barbara Eckmair[2]; Iain B. H. Wilson[2]; Katharina Paschinger[2]; [1]*Vetcore, Proteomics Facility, Veterinärmedizinische Universität Wien, Wien, Austria;* [2]*Department für Chemie, Universität für Bodenkultur, Wien, Austria*

HOMELAND SECURITY
MP 235-236

MP 235   **Detecting enzymatically active abrin and ricin toxins using MALDI**; Kaitlyn K. Drinkard[1]; Kaitlin Hoyt[1]; Susanne R. Kalb[1]; John R Barr[1]; [1]*Centers For Disease Control and Prevention, Atlanta, GA*

MP 236   **Improving the detection of molecular indicators of Abrus precatorius with LC-MS.**; Christina S Robb[1]; Kirk W Gaston[2]; Alexis G Mazurek[3]; [1]*The Connecticut Agricultural Experiment Station, New Haven, CT;* [2]*FDA Forensic Chemistry Center, Cincinnati, Ohio;* [3]*University of New Haven, New Haven, CT*

IMAGING MS: SAMPLE PREPARATION
MP 237-244

MP 237   **Matrix sublimation device with recristallization system for MALDI mass spectrometry imaging**; Vasiliy Eliferov[1]; Andrey Shivalin[1]; Daniil Ivanov[1]; Eugene (evgeny) Nikolaev[2]; Igor Popov[1]; [1]*Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation;* [2]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 238   **High resolution atmospheric-pressure mass spectrometry imaging of biological samples using a matrix-free ionization-assisting DIUTHAME foil**; Max Alexander Mueller[1]; Dhaka Ram Bhandari[1]; Kerstin Strupat[2]; Bernhard Spengler[1]; [1]*Justus Liebig University, Giessen, Germany;* [2]*Thermo Fisher Scientific, Bremen, Germany*

MP 239   **The utility of conductive adhesive film for the distribution analysis of small molecule by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Daisuke Saigusa[1]; Ritsumi Saito[1]; Komei Kawamoto[2]; Akira Uruno[1]; Kuniyuki Kano[1]; Junken Aoki[1]; Masayuki Yamamoto[1]; Tadafumi Kawamoto[2]; [1]*Tohoku University, Sendai, Japan;* [2]*Tsurumi University, Yokohama, Japan*

MP 240   **A new method for the robust localization and identification of proteins in mass spectrometry imaging of mineralized dental tissues**; Madeline Colley[1]; Sitai Liang[2]; Chunyan Tan[2]; Kyle P. Trobough[2]; Stephan B.H. Bach[3]; Yong-Hee Patricia Chun[2, 4]; [1]*University of Texas, San Antonio, TX;* [2]*UT Health San Antonio, Department of Periodontics, San Antonio, TX;* [3]*University of Texas in San Antonio, San Antonio, TX;* [4]*UT Health San Antonio, Department of Cell Systems and Anatomy, San Antonio, TX*

MP 242   **Improving molecular information provided by Mass Spectrometry Imaging of FFPE tissue**; Ekta Patel[1]; Kevin Randall[1]; Cathy Merry[2]; Philippa J Hart[1]; [1]*Medicines Discovery Catapult, Alderley Edge, United Kingdom;* [2]*University of Nottingham, Nottingham, United Kingdom*

MP 243   **Systematic Evaluation of Analyte Delocalization in Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging**; Eric S Barton[1]; Caitlin M. Tressler[2]; Kristine Glunde[2]; [1]*Johns Hopkins University School of Medicine, Baltimore, MD;* [2]*Johns Hopkins School of Medicine, Baltimore, MD*

MP 244   **Minimizing Visceral Fat Delocalization on Tissue Sections with Porous Aluminum Oxide Slides for Imaging Mass Spectrometry**; Frédéric Fournelle[1]; Ethan Yang[1]; Martin Dufresne[2]; Pierre Chaurand[1]; [1]*Department of Chemistry, University of Montreal,, Montréal, QC;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205*

IMAGING: FUNDAMENTALS **MP 245**	

MP 245	**The new gold standard for Mass Spectrometry Imaging**; Nolan K Mclaughlin[1]; Tyler Bielinski[1]; Katherine Stumpo[1]; [1]*University of Scranton, Scranton, PA*

INFORMATICS: GENERAL, SRM, AND DIA **MP 246-255**	

MP 246	**Prediction of peptide spectral libraries by deep learning and its use in proteomics**; Yi Yang[1]; Liang Qiao[1]; [1]*Fudan University, Shanghai, China*
MP 247	**Automated Screening of Modified 2′-Deoxynucleosides in Genomic DNA using a Custom Compound Discoverer 3.0 Node**; Scott J Walmsley[1, 2]; Nathaniel Mahieu[3]; Jingshu Guo[1, 4]; Haoqing Chen[1, 4]; Peter W. Villalta[1, 4]; Robert J. Turesky[1, 4]; [1]*Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Institute for Health Informatics, University of Minnesota, Minneapolis, MN; [3]Alethiun LLC, Centralia, MO; [4]Department of Medicinal Chemistry, College of Pharmacy, University of Minnesota, Minneapolis, MN*
MP 248	**Comparison of different processing pipelines for diaPASEF data**; Celine Henry[1]; Aaron Millan-Oropeza[1]; Stephanie Kaspar-Schoenefeld[2]; Schmit Pierre-Olivier[3]; Markus Lubeck[4]; Manuel Chapelle[3]; [1]*Université Paris-Saclay, INRAE, AgroParisTech, Micalis Institute, PAPPSO., Jouy-en-Josas, France; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, France; [4]Bruker Daltonics, Bremen, Germany*
MP 249	**Comparison of DDA and DIA Analysis of Complex Ocean Metaproteomics Samples and Targeted Metaproteomics to Estimate Biogeochemical Reaction Rates**; Mak Saito[1]; Brian Searle[2]; Matthew Mcilvin[1]; Jaclyn Saunders[1]; Dawn Moran[1]; [1]*Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; [2]Institute For Systems Biology, Seattle, WA*
MP 250	**TIMS-TOF Does DISCO: Spectrum-Driven DIA Analysis Software Tool (DISCO) is Amenable to TIMS-TOF PASEF DIA Data**; David D. Shteynberg[1]; Eric W. Deutsch[1]; Michael R. Hoopmann[1]; Luis Mendoza[1]; Mukul K. Midha[1]; Zhi Sun[1]; Samuel L. Bader[1]; Robert L. Moritz[1]; [1]*Institute For Systems Biology, Seattle, WA*
MP 251	**Matching peptides to data independent acquisition mass spectrometry data**; Yang Lu[1]; Wenruo Bai[1]; Jeffery A. Bilmes[1]; William Stafford Noble[1]; [1]*University of Washington, Seattle, WA*
MP 252	**Multi-Attribute-Method reporting with Panorama and Skyline**; Josh Eckels[1]; Nicholas Shulman[2]; Rich Rogers[3]; Haibo Qiu[4]; Yu Huang[4]; Ankur Juneja[1]; Sweta Jewargikar[1]; Bernard Lee[1]; Vagisha Sharma[2]; Michael J MacCoss[2]; Brendan Maclean[2]; [1]*LabKey, San Diego, CA; [2]University of Washington, Seattle, WA; [3]Bristol-Myers Squibb, Seattle, Washington; [4]Regeneron, Tarrytown, NY*
MP 253	**Skyline Support for Proteome-wide Data Analysis of Bruker timsTOF diaPASEF Acquisition**; Brian S. Pratt[1]; Matthew C Chambers[1]; Stephanie Kaspar-Schoenefeld[2]; Sven Brehmer[2]; Markus Lubeck[2]; Ute Distler[3]; Stefan Tenzer[3]; Michael J MacCoss[1]; Brendan Maclean[1]; [1]*Univ of Washington, Seattle, WA; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Institute for Immunology, University Medical Center Mainz, Mainz, Germany*
MP 254	**An update to Phosphomatics: A web resource for phosphoproteome analysis**; Michael G Leeming[1]; Sean O'callaghan[2]; Luana Licata[3]; Marta Iannuccelli[3]; Prisca Lo Surdo[3]; Elisa Micarelli[3]; Ching-Seng Ang[1]; Shuai Nie[1]; Swati Varshney[1]; Sadia Ameen[1]; Heung-Chin Cheng[1]; Nicholas A Williamson[1]; [1]*University of Melbourne, Melbourne, Australia; [2]Nuritas Limited, Dublin, Ireland; [3]University of Rome Tor Vergata, Rome, Italy*
MP 255	**PINE: An Automation Tool to Extract & Visualize Protein-Centric Functional Networks**; Niveda Sundararaman[1]; James Go[1]; Aaron Robinson[1]; Jose Mato[2]; Shelly C. Lu[3]; Jennifer E Van Eyk[1]; Vidya Venkatraman[1]; [1]*Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; [2]CIC bioGUNE, Centro de Investigación Biomédica en Red de Enfermedades Hepáticas y Digestivas (Ciberehd), Derio, Spain; [3]Division of Digestive and Liver Diseases, Cedars-Sinai Medical Center, Los Angeles, CA*

INFORMATICS: METABOLOMICS **MP 256-275**	

MP 256	**High-Throughput Metabolite Profiling for Synthetic Biology using Ion Mobility-Mass Spectrometry and Data-Independent Acquisition with Improved Targeted Data Extraction Software**; Aivett Bilbao[1]; Nathalie Munoz[1]; Daniel J. Orton[1]; Xueyun Zheng[1]; Karl K. Weitz[1]; Kyle Pomraning[2]; Shuang Deng[1]; Beth Hofstad[2]; Ziyu Dai[2]; Alex Apffel[3]; Richard D. Smith[1]; Young-Mo Kim[1]; Jon Magnuson[2]; Kristin E. Burnum-Johnson[1]; [1]*Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington; [2]Chemical and Biological Processes Development Group, Richland, Washington; [3]Agilent Technologies, Santa Clara, CA*
MP 257	**Exploring DIA data analysis for metabolomics with Spectronaut**; Maximilian J. Helf[1]; Kathleen Rousseau[2]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; François Fenaille[2]; Lukas Reiter[1]; [1]*Biognosys, Schlieren, Switzerland; [2]Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France*

MP 258 **Fingerprint-decoding neural networks enable database-independent compound generation from fragment spectra**; <u>Michael Andrej Stravs</u>[1, 2]; Kai Dührkop[3]; Heinz Singer[2]; Sebastian Böcker[3]; Nicola Zamboni[1]; [1]*ETH Zurich, Zurich, Switzerland;* [2]*EAWAG, Duebendorf, Switzerland;* [3]*Friedrich-Schiller University of Jena, Jena, Germany*

MP 259 **Comparing accurate mass MS/MS spectral similarity algorithms for small molecules**; <u>Yuanyue Li</u>[1]; Tobias Kind[1]; Oliver Fiehn[1]; [1]*NIH West Coast Metabolomics Center, UC Davis, Davis, California*

MP 260 **Mass spectrometry searches using MASST**; <u>Mingxun Wang</u>[1, 2]; Alan K. Jarmusch[1]; Fernando Vargas[1]; Alexander A. Aksenov[3]; Julia M. Gauglitz[1]; Kelly Weldon[1]; Daniel Petras[1]; Ricardo Silva[1]; Robert Quinn[4]; Alexey Melnik[1]; Justin Van Der Hooft[5]; Andres Caraballo-Rodriguez[1]; Louis-Felix Nothias[1]; Christine Aceves[1]; Morgan Panitchpadki[1]; Elizabeth Brown[1]; Francesca Di Ottavio[1]; Nicole Sikora[1]; Emmanuel Elijah[1]; Lara Labarta-Bajo[1]; Emily Gentry[1]; Shabnam Shalapour[1]; Kathleen Kyle[6]; Sara Puckett[6]; Jeramie Watrous[1]; Carolina Carpenter[1]; Amina Bouslimani[1]; Madeleine Ernst[1]; Austin Swafford[1]; Elina Zuniga[1]; Marcy Balunas[6]; Johnathan Klassen[6]; Rohit Loomba[1]; Rob Knight[1]; Nuno Bandeira[1]; Pieter C. Dorrestein[1]; [1]*UCSD, La Jolla, CA;* [2]*Ometa Labs, San Diego, CA;* [3]*Collaborative Mass Spectrometry Innovation Center, University of California San Diego, La Jolla, CA;* [4]*Michigan State University, East Lansing, MI;* [5]*Wageningen University and Research, Wageningen, Netherlands;* [6]*University of Connecticut, Storrs, CT*

MP 261 **Crossing the Chasm:One integrated solution for advancing LC-PASEF based pharma, metabolomics, non-target screening and exposome research**; <u>Xuejun Peng</u>[1]; Guillaume Tremintin[1]; Heiko Neuweger[2]; Aiko Barsch[2]; Heino M. Heyman[3]; Sofie Weinkouff[2]; Nikolas Kessler[2]; [1]*Bruker Daltonics, San Jose, CA;* [2]*Bruker Daltonik GmbH, Bremen, Germany;* [3]*Bruker Daltonics, Billerica, MA*

MP 262 **Combining Chromatographic Deconvolution with Electron Ionization and Chemical Ionization for Unknown Identification with High-Resolution Accurate Mass GC/MS**; Dominic Roberts[1]; <u>Jason Cole</u>[2]; Xin Zheng[2]; John Voss[2]; [1]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [2]*Thermo Fisher Scientific, Austin, TX*

MP 263 **molDiscovery: learning mass spectrometry fragmentation**; <u>Liu Cao</u>[1]; Alexey Gurevich[2]; Hosein Mohimani[1]; [1]*Carnegie Mellon University, Pittsburgh, PA;* [2]*St. Petersburg State University, St. Petersburg, Russia*

MP 264 **MetaboDashboard: A simple machine learning pipeline and visualisation tool for metabolomics applied to diet profiles**; Francis Briere[1]; <u>Nancy Boucher</u>[2]; Pier-Luc Plante[1]; Jacques Corbeil[1, 2]; Didier Brassard[3]; Benoit Lamarche[3]; [1]*Université Laval, Québec, QC;* [2]*CHU de Québec-Université Laval, Quebec, Qc;* [3]*Institute of Nutrition and Functional Foods, Quebec, Qc*

MP 265 **Automated Metabologenomics Pipeline for Scalable Non-Ribosomal Peptide (NRP) Discovery Finds NRPs Produced by Soil and Human Skin Microbes**; <u>Bahar Behsaz</u>[1]; Alexey Gurevich[2]; Amina Bouslimani[3]; Rob Knight[3]; Pieter C. Dorrestein[3]; Hosein Mohimani[4]; Pavel A. Pevzner[3]; [1]*UC San Diego, La Jolla, CA;* [2]*St. Petersburg State University,, St. Petersburg, Russia;* [3]*University of California San Diego, San Diego, CA;* [4]*Carnegie Mellon University, Pittsburgh, PA*

MP 266 **An underappreciated challenge in identifying metabolites: scoring matches between library spectra and LC-MS HRAM metabolite spectra from complex samples**; <u>Lewis Y. Geer</u>[1]; Yamil Simón-Manso[1]; Xiaoyu Yang[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

MP 269 **mzRAPP – enabling routine performance checks of non-targeted data pre-processing in LC-HRMS**; <u>Yasin El Abiead</u>[1, 2, 3]; Maximilian Milford[1]; Gunda Koellensperger[1, 2, 3]; [1]*University of Vienna, Department of Analytical Chemistry, Vienna, Austria;* [2]*Chemistry meets Microbiology, University of Vienna, Vienna, Austria;* [3]*Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria*

MP 270 **In-source CID ramping (InCIDR) and Co-variant ion analysis of hydrophilic interaction chromatography (HILIC) metabolomics**; Eric Chiles[1]; Sara Maimouni[1]; Fredric E. Wondisford[1]; Wei-Xing Zong[1]; Chi Song[2]; <u>Xiaoyang Su</u>[1]; [1]*Rutgers University, New Brunswick, NJ;* [2]*The Ohio State University, Columbus, OH*

MP 271 **PAVE: an isotope labeling-based peak annotation engine for microbial metabolomics data analysis**; <u>Wenyun Lu</u>[1]; Lin Wang[1]; Xi Xing[1]; Li Chen[1]; Joshua D. Rabinowitz[1]; [1]*Princeton University, Princeton, NJ*

MP 272 **SIRIUS 4: A fully automated workflow from feature detection to compound identification**; Martin A Hoffmann[1]; <u>Kai Dührkop</u>[2]; Marcus Ludwig[1]; Markus Fleischauer[2]; Sebastian Böcker[2]; [1]*Friedrich-Schiller-University Jena, Jena, Germany;* [2]*Friedrich-Schiller University of Jena, Jena, Germany*

MP 273 **Considerations in the chromatographic processing of >100,000 retention indexed plant metabolomics GC-MS files by Genedata Expressionist**; <u>Brian M. Ruddy</u>[1]; Joseph D. Shambaugh[2]; David A. Curiel[1]; Teresa K. Harp[1]; Jan P. Hazebroek[1]; [1]*Corteva Agriscience, Johnston, IA;* [2]*Genedata, Lexington, MA*

MP 274 **Polly-PeakML: Uncovering the dark-matter of metabolomic space using a novel machine-learning algorithm for peak classification**; Richa Mudgal[1]; Kailash Yadav[1]; Sailful Bari Khan[1]; Shashank Jatav[1]; Kelly Marsh[2]; Brian Dranka[3]; <u>Abhishek Jha</u>[3]; [1]*Elucidata, Delhi, India;* [2]*Agios Pharmaceuticals, Inc., Cambridge, MA;* [3]*Elucidata, Cambridge, MA*

MP 275 **SIFTER: Chemical Class Prediction of Unknown Biomolecules Using Ion Mobility-Mass Spectrometry and Machine Learning**; <u>Jaqueline A. Picache</u>[1]; Jody C. May[1]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN*

INSTRUMENTATION: GENERAL
MP 276-290

MP 276   **Biological Detection by Trapped Particle Fluorescence**; Nathan a Grimes[1]; Theresa Nguyen[2]; [1]*University of South Florida, Tampa, FL;* [2]*University of South Florida, Tampa*

MP 277   **Quantitation of microparticles through a quadrupole-ion-trap mass spectrometer**; Chun-Jen Hsiao[1]; Jung-Lee Lin[1]; Abdil Özdemir[2]; Chung-Hsuan Chen[1]; [1]*Academia Sinica, Taipei, Taiwan;* [2]*Sakarya university, Adapazarı, Turkey*

MP 278   **Raising the mass limit for determination of collision cross sections of proteins and protein complexes using an Orbitrap mass spectrometer**; James D. Sanders[1]; Virginia K. James[1]; Konstantin Ayzikov[2]; Kyle L. Fort[2]; Dmitry Grinfeld[2]; Alexander Makarov[2]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*Thermo Fisher Scientific, Bremen, Germany*

MP 279   **Resonance-Enhanced Detection of Metals in Aerosols using Single Particle Mass Spectrometry**; Sven Ehlert[1, 2]; Johannes Passig[2, 3, 4]; Julian Schade[2, 4]; Ellen Iva Rosewig[2, 4]; Robert Irsig[1, 2]; Thomas Kröger-Badge[2, 4]; Hendryk Czech[2, 3]; Martin Sklorz[3]; Thorsten Streibel[2, 3]; Lei Li[5]; Zhen Zhou[5]; Xue Li[5]; Henrik Fallgren[6]; Jana Moldanova[6]; Stefan Zimmermann[2, 3]; [1]*Photonion GmbH, Schwerin, Germany;* [2]*Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University Rostock, Rostock, Germany;* [3]*Joint Mass Spectrometry Centre, Cooperation Group Comprehensive Molecular Analytics (CMA), Helmholtz Zentrum München, Neuherberg, Germany;* [4]*Department Life, Light & Matter, University of Rostock, Rostock, Germany;* [5]*Hexin Instrument Co., LTD, Guangzhou, China;* [6]*IVL Swedish Environmental Research Institute, Gothenburg, Sweden*

MP 280   **Numerical and experimental investigation of an rf-ion funnel**; Laurent Bernier[1]; Loukas Kyriakidis[1]; Philipp Krah[1]; Paul Fremdling[2]; Stephan Rauschenbach[2]; Julius Reiss[1]; [1]*Technical University Berlin, Berlin, Germany;* [2]*University of Oxford, Oxford, United Kingdom*

MP 281   **Highly flexible experiment design using XML control of a Q-cyclic IMS-ToF**; Jason L Wildgoose[1]; James I Langridge[1]; Darren Hewitt[1]; Paul Doorbar[1]; David Harker[1]; Konstantinos Thalassinos[2, 3]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*University College London, London, United Kingdom;* [3]*Birkbeck College, University of London, London, United Kingdom*

MP 282   **Development of Quadrupole Ion Simulation Using Python**; Jake Connolly; *Bruker Daltonics, Billerica, MA*

MP 283   **Determination of contaminants when calibrating an Orbitrap Mass Spectrometer And How to Avoid Them**; David Bergen[1]; Michael Goodwin[1]; Helene Cardasis[1]; Jesse D Canterbury[1]; Graeme Mcalister[1]; Michael W. Senko[1]; Shannon Eliuk[1]; Vlad Zabrouskov[1]; Romain Huguet[1]; [1]*Thermo Fisher Scientific, San Jose, California*

MP 284   **Improve the sensitivity of haloacetic acids and phenols by increasing ion transmittance of an ion guide at higher pressure vacuum**; Manabu Ueda[1]; Takanari Hattori[1]; Wataru Fukui[1]; Tsubasa Ibushi[2]; Kazuo Mukaibatake[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Shimadzu Techno-Research, Inc., Kyoto, Japan*

MP 285   **Origins and mitigation of unwanted dissociation of fragile analyte ions in compact quadrupole Orbitrap mass spectrometers**; Erik P.A. Couzijn[1]; Siegrun A.I. Mohring[1]; Ioanna Ntai[2]; Jan-Peter Hauschild[1]; Alexander Harder[1]; Alexander A. Makarov[1]; [1]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [2]*Thermo Fisher Scientific, San Jose, CA*

MP 286   **A tandem instrument for travelling-wave ion mobility separation and direct collision cross-section determination**; Jakub Ujma[1]; Kevin Giles[1]; Jason L Wildgoose[1]; David Langridge[1]; Keith Richardson[1]; Alistair Schofield[1]; Witold Niklewski[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

MP 287   **A Proteomic Sample Preparation for Mass Spectrometry Using an Automated Workstation**; Qin Fu[1]; Casey W Johnson[1]; Bhagya K Wijayawardena[2]; Michael P Kowalski[2]; Miranda Kheradmand Kheradmand[2]; Jennifer E Van Eyk[1]; [1]*Cedars Sinai Medical Center, Los Angeles,, CA;* [2]*Beckman Coulter Life Sciences, San Jose, CA*

MP 288   **Bond Dissociation Calculations to Evaluate Molecular Fragmentation Caused by Hypervelocity Impacts in Closed-Source Mass Spectrometers**; Brandon Turner[1]; Daniel E. Austin[1]; Eric T. Sevy[1]; [1]*Brigham Young University, Provo, UT*

MP 289   **New sample delivery and automation methods enable microsecond measurements in the X-ray footprinting mass spectrometry experiment**; Sayan Gupta[1]; Line Kristensen[2]; Daniel P Deponte[3]; Matthew Rosi[4]; Brandon Russell[4]; Erik Farquhar[5]; Michael Sullivan[5]; Donald Abel[5]; Rohit Jain[6]; Shawn Costello[7]; Yan Chen[2]; Mark R. Chance[6]; Christopher J. Petzold[8]; Farid Farahmand[4]; Corie Y Ralston[9]; [1]*Lawrence Berkeley National Laboratory, Berkeley, California;* [2]*Lawrence Berkeley Laboratory, University of California, Berkeley, California;* [3]*SLAC National Accelerator Laboratory, Standford, California;* [4]*Sonoma State University, Rohnert Park, California;* [5]*Brookhaven National Laboratory, Upton, NY;* [6]*Case Western Reserve University, Cleveland, OH;* [7]*University of California, Berkeley, Berkeley, CA;* [8]*Lawrence Berkeley National Laboratory, Berkeley;* [9]*Lawrence Berkeley National Laboratory, Berkeley, CA*

MP 290   **Glow Flow: a step towards a universal ion source**; Rhodri N. Owen[1]; Steve L Kelly[1]; Gareth Brenton[1]; [1]*Swansea University, Swansea, United Kingdom*

ION MOBILITY: FAIMS/DMS
MP 291-295

MP 291   **Low-Field Differential Ion Mobility Spectrometry of Dipole-Aligned Macromolecules**; Pratima Pathak[1]; Alexandre Shvartsburg[1]; [1]*Wichita State University, Wichita, KS*

MP 292   **Distinguishing Unique Conformers of Monosaccharides using Differential Ion Mobility Spectrometry-Mass Spectrometry (DIMS-MS)**; Tiffany L Crawford[1]; Gary L Glish[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 293   **Pre-filtration and separation of drug isomer pairs using Differential mobility spectrometry-mass spectrometry (DMS-MS)**; Ifeoluwa Ayodeji[1]; Linxia Song[2]; Kenyon Evans-Nguyen[3]; Theresa Evans-Nguyen[2]; [1]*University of South Florida, Tampa, FL; [2]University of South Florida, Tampa; [3]University of Tampa, Tampa, FL*

MP 294   **Proteomic analysis and isobaric separation using FAIMS interfaced mass spectrometry**; Laxmi Sinduri Vuppala[1]; Theresa Evans-Nguyen[1]; Petra Mick[1]; Mahitha Nuthulaganti[1]; [1]*University of South Florida, Tampa*

MP 295   **Protonation isomers of highly charged protein ions can be separated in FAIMS-MS**; J. Diana Zhang[1]; Micah T. Donor[2]; Amber D. Rolland[2]; James S. Prell[2]; William A. Donald[1]; [1]*University of New South Wales, Sydney, Australia; [2]University of Oregon, Oregon, Oregon*

ION MOBILITY: FUNDAMENTALS
MP 296-309

MP 296   **The Inelasticity of Ion-Molecule Collisions in Ion Mobility Spectrometry**; Glenn E. Spangler; *Technispan LLC, Lutherville, MD*

MP 297   **Effect of acetonitrile vapor in the ESI source on protomer distribution of protonated para-aminobenoic acid (PABA)**; Zhaoyu Zheng[1]; Athula B. Attygalle[2]; [1]*Stevens Institute of Technology, Jersey City, NJ; [2]Stevens Institute of Technology, Hoboken, NJ*

MP 298   **Collision Cross Section Calibration Strategies for a Prototype SLIM-based Ion Mobility Instrument**; Bailey S. Rose[1]; Katrina L. Leaptrot[1]; Kelly L. Wormwood Moser[2]; Jody C. May[1]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN; [2]Mobilion Systems, Inc., Chadds Ford, PA*

MP 299   **Investigations on the formation of positive and negative reactant ions in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) by HiKE-IMS-MS**; Maria Allers[1]; Ansgar T. Kirk[1]; Duygu Erdogdu[2]; Robin Hillen[2]; Walter Wissdorf[2]; Thorsten Benter[2]; Stefan Zimmermann[1]; [1]*Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany; [2]University of Wuppertal, Wuppertal, Germany*

MP 300   **Chemical Reaction and Transport Simulations of Positive Reactant Ions in High Kinetic Energy IMS (HiKE-IMS)**; Duygu Erdogdu[1]; Maria Allers[2]; Walter Wissdorf[1]; Clara Markert[1]; Hendrik Kersten[1]; Stefan Zimmermann[2]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany; [2]Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany*

MP 301   **PhaseCRAFTI: a New Approach to Collision Cross Section Measurements Using FTICR/MS Phase Shifts**; David V. Dearden[1]; Matthew C. Asplund[1]; Andrew J. Arslanian[1]; Tina H. M. Farzan[1]; Jamir Shrestha[1]; [1]*Brigham Young University, Provo, UT*

MP 302   **Compact HiKE-IMS for Quantitative Trace Gas Detection in Field Applications**; Florian Schlottmann[1]; Ansgar T. Kirk[1]; Alexander Bohnhorst[1]; Maria Allers[1]; Christoph Schaefer[1]; Sebastian Kehlenbeck[1]; Alexander Schwarz[1]; Bert Ungethuem[2]; Falko Ziegert-Kuehn[2]; Andreas Walte[2]; Stefan Zimmermann[1]; [1]*Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Hannover, Germany; [2]AIRSENSE Analytics GmbH, Schwerin, Germany*

MP 303   **Tandem DT-IMS/TIMS-MS for Accurate Mobility Measurements**; Kim Q Dang[1]; Francisco Fernandez-Lima[2]; [1]*FIU, Miami, FL; [2]Florida International University, Miami, Florida*

MP 304   **Accurate Modeling of Peak Shapes and Drift Times in SLIM Traveling Wave Ion Mobility Spectrometry**; Sidney E. Buttrill, Jr. [1]; Daniel Debord[2]; Liulin Deng[2]; [1]*Consultant, Palo Alto, CA; [2]MOBILion Systems Inc., Chadds Ford, PA*

MP 305   **Optimization of tristate gating and multiplexing parameters for improved ion mobility mass spectrometry of biomolecules**; Jamie P Butalewicz[1]; James D. Sanders[1]; Virginia K. James[1]; Brian H Clowers[2]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX; [2]Washington State University, Pullman, WA*

MP 306   **Identifying the role of proton transfer reactions for proteins in the gas phase**; Tyler C Cropley[1]; Mengqi Chai[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

MP 307   **Investigation of Resveratrol Photoisomerization Product by Ultra-Performance Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry (UPLC-IMS-MS)**; Gabriella V Litterio[1]; Sihang Xu[1]; Athula B. Attygalle[1]; [1]*Stevens Institute of Tecnology, Hoboken, NJ*

MP 308 **Propagating error associated with TWIMS calibrations increases the accuracy of calculated CCS values**; Alexis N. Edwards[1]; Hien M. Tran[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

MP 309 **Inadequacies of common theoretical and numerical tools to predict ion-mobilities on-par with high-resolution experimental observations and how to overcome them**; Carlos Larriba Andaluz[1]; Viraj Gandhi[1, 2]; *[1]IUPUI, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

ISOTOPE LABELING AND FLUXOMICS APPLICATIONS
MP 310-314

MP 310 **Hypothesis driven computational analysis of isotope tracer studies**; Ethan Stancliffe[1, 2]; Michaela Schwaiger-Haber[1]; Miriam Sindelar[1]; Gary J. Patti[1, 2]; *[1]Department of Chemistry, Washington University in St. Louis, St. Louis, MO; [2]Department of Medicine, Washington University in St. Louis, St. Louis, MO*

MP 311 **Cancer detection using 13C tracing and liquid biopsy**; Likun Duan[1]; Grace Scheidemantle[1]; Xiaojing Liu[1]; *[1]North Carolina State University, Raleigh, NC*

MP 312 **DiLeuPMP: a multiplexed isobaric labeling method for high-throughput quantitative analysis of O-glycans**; Ting-Jia Gu[1]; Miyang Li[2]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*

MP 314 **Integrating MetaboScape and PollyTMfor the analysis of LC-TIMS-MS and LC-MS based fluxomics**; Heino M. Heyman[1]; Heiko Neuweger[2]; Pawel Konrad Lorkiewicz[3]; Bradford G. Hill[3]; Kyle Fulghum[3]; Shefali Lathwal[4]; Avijit Zutshi[5]; Brian Dranka[6]; Swetabh Pathak[5]; Abhishek Jha[6]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]University of Louisville, Louisvlille, KY; [4]Elucidata, New Delhi, India; [5]Elucidata, Delhi, India; [6]Elucidata, Cambridge, MA*

LC/MS: GENERAL
MP 315-332

MP 315 **Development of a LC-MS/MS method for simultaneously determination of 30 pesticides in Chenpi**; Xin Zheng[1]; Yueqi Li[1]; Taohong Huang[2]; *[1]Shimadzu(China) Co.,LTD.Beijing Branch, Beijing, China; [2]Shimadzu (China) Co., Ltd, Shanghai, China*

MP 316 **Development of a LC/MS Single Quadrupole Workflow for Mapping the Binding Site of Peptidomimetic Probes**; Christine S Muli; *Purdue University, West Lafayette, IN*

MP 317 **Monitoring of on-column methionine oxidation as part of a system suitability test during UHPLC-MS/MS peptide mapping**; Vincent Larraillet[1]; Björn Mautz[1]; Maximiliane Koenig[1]; Michael Molhoj[1]; *[1]Roche Pharma Research and Early Development, Roche Innovation Center Munich, Germany*

MP 318 **Trace analysis oTrace analysis of abused drugs in waste water sample by AOE system coupled with LCMS-8060**; Jiaqi Liu[1]; Yunzhong Zheng[1]; Qisheng Zhong[1]; Taohong Huang[2]; *[1]Shimadzu (China) Co., LTD. Guangzhou Branch, Guangzhou, China; [2]Shimadzu (China) Co., Ltd., Shanghai Office, Shanghai, China*

MP 319 **Transferring metabolomics methods from high-resolution Orbitrap to triple quadrupole mass spectrometers**; Michaela Schwaiger-Haber[1]; Ethan Stancliffe[1, 2]; Miriam Sindelar[1]; Gary J. Patti[1, 2]; *[1]Department of Chemistry, Washington University in St. Louis, St. Louis, MO; [2]Department of Medicine, Washington University in St. Louis, St. Louis, MO*

MP 320 **Metabolic changes related to the IDH1 mutation in gliomas preserve TCA-cycle activity**; Theo Luider; *Erasmus MC, Rotterdam, Netherlands*

MP 321 **Developing a Qualified Total Antibody and Antibody-Conjugated Drug Assay for In Vitro Plasma Stability Study**; Elena Ter-Ovanesyan[1]; Ling Xu[1]; David H Lee[1]; *[1]Mersana Therapeutics, Cambridge, MA*

MP 322 **LC/MS analysis of phosphorothioate oligonucleotides using a polymer-based HILIC column having diol group**; Leah Sullivan; *Shodex, Showa Denko America, Inc., New York, NY*

MP 323 **Mass Spectrometric characterization of the glycoform peaks of monoclonal antibodies separated by a novel FcR analytical affinity chromatography column**; Atis Chakrabarti; *Tosoh Bioscience LLC, King Of Prussia, PA*

MP 325 **Comprehensive Phytochemical Evaluation of White Unaged and Aged Allium sativum by LC-ESI-MS/MS; A comparative Study**; Mustafa Abdullah Yilmaz[1]; Abdulselam Ertas[1]; Oguz Cakir[1]; Ismail Yener[1]; Hamdi Temel[1]; *[1]Dicle University, Diyarbakir, Turkey*

MP 326 **Decellularized Extracellular Matrix Components Drive Cardiac Fate: Cues from Matrisome Influence Atrial Differentiation**; Fernanda C P Mesquita[1]; Po-Feng Lee[1]; Yutao Xi[1]; Jacquelynn Morrissey[1]; Helen Andersson[1]; Gustavo Monnerat[2]; Fabio CS Nogueira[2]; Gilberto Domont[2]; Luiz C Sampaio[1]; Camila Hochman-Mendez[1]; Doris A Taylor[1]; *[1]Texas Heart Institute, Houston, TX; [2]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*

MP 327 **Development of a sensitive LC-MS/MS Method for the Quantification of a Stereopure Phosphorothioate Antisense Oligonucleotide in Human Plasma**; <u>Andrew Hart</u>[1]; Susovan Mohapatra[1]; Esme Candish[2]; Ji Jiang[2]; [1]*Wave Life Sciences, Lexington, MA;* [2]*Sciex, Framingham, MA*

MP 328 **Trace-level quantitative analysis of Poloxamers in biological samples by HPLC-ESI-QqQ MS**; <u>Ali Najafi</u>[1]; Neelanjan Bose[1]; [1]*Emery Pharma, Alameda, CA*

MP 329 **Simplified high-throughput methods for deep and targeted proteome analysis on thetimsTOFPro**; <u>Jarrod J Sandow</u>[1, 2, 3]; Giuseppe Infusini[1, 2, 3]; Michael Krawitzky[4]; Christopher Adams[4]; Laura Dagley[1, 2]; Rune Larsen[1, 2]; Andrew I Webb[1, 2, 3]; [1]*The Walter & Eliza Hall Institute, Parkville, Australia;* [2]*University of Melbourne, Parkville, Australia;* [3]*IonOpticks, Fitzroy, Australia;* [4]*Bruker Daltonics, San Jose, CA*

MP 330 **Effect of Vancomycin on Cytoplasmic Peptidoglycan Intermediate Levels In Resistant Enterococcus faecium**; <u>Shivani Gargvanshi</u>; *University of Missouri-Kansas City, Kansas City, MO*

MP 331 **Metabolomics reveals a correlation between hydroxyeicosatetraenoic acids and allergic asthma in children: evidence from three years of immunotherapy**; <u>Jian-lin Wu</u>[1]; Na Li[2]; [1]*Macau University of Science and Technology, Macau, Macau;* [2]*Macau University of Science and Technology, Macao, Macau, Macao*

MP 332 **Expanding the versatility of the Evosep One with a toolbox of specialized workflows for MS-based omics**; Dorte B. Bekker-Jensen[1]; Ole B. Horning[1]; Andreas-David Brunner[2]; Catherine G. Vasilopoulou[2]; Florian Meier[2]; Philipp E. Geyer[2]; Peter A. Nielsen[1]; Lasse Falkenby[1]; Jesper V. Olsen[3]; Ole Vorm[1]; Matthias Mann[2]; <u>Nicolai Bache</u>[1]; [1]*Evosep Biosystems, Odense, Denmark;* [2]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [3]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

LC/MS: SAMPLE PREPARATION I
MP 333-351

MP 333 **Automating the Preparation of Matrix Matched Calibration Standards for the Analysis of Food Contaminants by LC/MS/MS**; <u>Fred Foster</u>[1]; John Stuff[1]; Laurel Vernarelli[1]; Jacqueline Whitecavage[1]; [1]*Gerstel, Inc., Linthicum, MD*

MP 334 **Evaluation of sample preparation workflows for proteomics analysis of Chlamydomonas reinhardtii**; <u>Shin-Cheng Tzeng</u>[1]; Ningning Zhang[1]; Ru Zhang[1]; Bradley Evans[1]; [1]*Donald Danforth Plant Science Center, Saint Louis, MO*

MP 335 **Steroid Screening in Horse Plasma via 96-Well Plate Supported Liquid Extraction**; <u>Deidre E. Damon</u>[1]; Mohamed Youssef[2]; [1]*Ohio Department of Agriculture, Reynoldsburg, OH;* [2]*Biotage, Charlotte, North Carolina*

MP 336 **Evaluation of trypsin activity through accelerated protein digestion at elevated temperatures**; <u>Alan A. Doucette</u>[1]; Jessica Nickerson[1]; [1]*Dalhousie University, Halifax, NS*

MP 337 **Time and Money Savings by the Implementation of Automated µSPE for Cleanup of QuEChERS Extracts of Veterinary Drugs**; <u>Jonathan Beck</u>[1]; Tom Flug[1]; Laura E Burns[2]; Dwayne E Schrunk[2]; Dipankar Ghosh[3]; Ed George[3]; [1]*CTC Analytics AG, Lake Elmo, MN;* [2]*Iowa State University, Ames, IA;* [3]*Thermo Fisher Scientific, San Jose, CA*

MP 339 **New Stop And Go Extraction Tips applied on peptidic purification and comparison with two other SPE tips from different manufacturer**; <u>Sami Bayoudh</u>[1]; Mohamed Amine Ben Mlouka[2]; Pascal Cosette[2]; Julie Hardouin[2]; Kaynoush Naraghi[1]; Corentin Germain[1]; Michel Arotcarena[1]; [1]*AFFINISEP, Petit Couronne, France;* [2]*PISSARO Proteomic Facility, IRIB, Mont-Saint-Aignan, France*

MP 340 **Evaluation of a Novel Low-Volume 96-well SPE Format for Forensic and Clinical Toxicology prior to UHPLC-MS/MS Analysis**; <u>Lee Williams</u>[1]; Geoff Davies[1]; Katie-Jo Teehan[1]; Adam Senior[1]; Alan Edgington[1]; Helen Lodder[1]; [1]*Biotage GB Limited, Cardiff, United Kingdom*

MP 341 **Use of immobilized trypsin in proteomic workflows enables full automation and reduces undesirable by-products**; <u>Patrick Kates</u>[1]; B. Todd Mullis[2]; Michael Walla[2]; William Cotham[2]; Qian Wang[2]; L. Andrew Lee[1]; [1]*Integrated Micro-chromatography Systems, Inc, Irmo, SC;* [2]*University of South Carolina, Columbia, SC*

MP 342 **Development of an Ultracentrifugation Method to Determine Etrasimod (APD334) Human Plasma Protein Binding (PPB) at Clinically Relevant Plasma Concentration**; <u>Michae G. Ma</u>[1]; Kelem Kassahun[2]; Rostislav Kuskovsky[2]; Yong Q. Tang[1]; Caroline A. Lee[1]; John S. Grundy[1]; [1]*Arena Pharmaceuticals, San Diego, CA;* [2]*Frontage Laboratories, Inc., Exton, PA*

MP 343 **EasyPep Sample Preparation Technology for Rapid and Efficient Mass Spectrometry-based Proteomics**; Sergei Snovida[1]; <u>Amarjeet Flora</u>[1]; Bhavin Patel[2]; Penny Jensen[2]; Ryan Bomgarden[2]; [1]*Thermo Fisher Scientific, Rockford, IL;* [2]*ThermoFisher Scientific, Rockford, IL*

MP 344 **Determination of Zoledronic Acid in Dog Serum by LC-MS/MS Xiaohua Li, Allan Xu1, 1Keystone Bioanalytical, Inc.**; <u>Allan Xu</u>; *Keystone Bioanalytical, North Wales, PA*

MP 345 **Analysis of Per- and Polyfluoroalkyl Substances in Drinking Water Using EPA Methods 533, 537.1 with Semi-Automated Solid Phase Extraction (EZPFC™)**; Ruud Addink[1]; Tom Hall[1]; [1]*Fluid Management Systems, Watertown, MA*

MP 346 **Assessing in-vivo stability of a pretargeted, bioorthogonal anti-sense oligonucleotide using click chemistry tools, a one-step SPE, and LC-MS/MS**; Stanley Goldstein[1]; Pei Li[1]; Brendon E. Cook[1]; [1]*Biogen, Cambridge, MA*

MP 347 **Si-Trap: simultaneous, high throughput multiomics sample preparation**; John Wilson[1]; Alexandre Zougman[2]; Lee D. Roberts[3]; Rosamonde E. Banks[2]; [1]*ProtiFi, LLC, Huntington, NY; [2]University of Leeds, Leeds, United Kingdom; [3]Leeds Institute of Cardiovascular and Metabolic Medicine, University of Leeds, Leeds, United Kingdom*

MP 348 **Automation of Sample Preparation and Buffer Exchange for Multi-Attribute Method**; P. Nikki Sitasuwan[1]; Thomas W. Powers[2]; Tiffany Medwid[2]; Yuko Ogata[3]; Nancy S Nightlinger[3]; Richard S Rogers[4]; Casey Snodgrass[5]; Pamela Quizon[1]; L. Andrew Lee[1]; [1]*Integrated Micro-chromatography Systems, Inc, Irmo, SC; [2]Pfizer Inc., Chesterfield, MO; [3]Just - Evotec Biologics, Seattle, WA; [4]Bristol-Myers Squibb, Seattle, Washington; [5]Hamilton Company, Reno, NV*

MP 349 **Development and application of a novel thin film molecularly imprinted polymer for the measurement of mycophenolic acid in human plasma**; Evan Langille[1]; Fereshteh Shahhoseini[1]; Ali Azizi[1]; Christina Bottaro[1]; [1]*Memorial University, St. John's, NL*

MP 350 **An automated LC-MS sample preparation workflow for the characterization of recombinant monoclonal antibodies using a benchtop pipetting robot**; Aarti Jashnani[1]; Srikanth Kotapati[1]; Jason Hogan[1]; Gavin Dollinger[1]; [1]*Bristol-Myers Squibb, Redwood City, CA*

MP 351 **Thin film molecularly imprinted polymers (TF-MIPs) for reliable single-use microextraction devices for selective enrichment of organophosphorus pesticides**; Ali Azizi[1]; Fereshteh Shahhoseini[1]; Evan Langille[1]; Christina Bottaro[1]; [1]*Memorial University, St. John's, NL*

LIPIDS: GENERAL
MP 352-367

MP 352 **Integrating Hydrophilic Interaction Chromatography, Trapped Ion Mobility Spectrometry, and Isomer Resolving MS/MS for In-Depth Lipidomic Profiling**; Tian Xia[1]; Hengxue Shi[1]; Yu Xia[1]; [1]*Tsinghua University, Beijing, China*

MP 353 **Effect of Leishmania donovaniinfection on the lipidome and metabolome of RAW264.7 macrophage-derived exosomes**; Andrew P Kurland[1]; Anna Gioseffi[1]; Peter Kima[1]; Timothy J Garrett[1]; [1]*University of Florida, Gainesville, FL*

MP 354 **MALDI-MS, MS/MS and MALDI imaging of triple-negative breast cancers identified novel phospholipid cell membrane alterations involved in tumor progression regulation**; Dilrukshika S. W. Palagama[1]; Brock A Humphries[1]; Jagadish Boppisetti[1]; Youngsoon Jang[1]; Brian D Ross[1]; Gary D Luker[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 355 **Hepatic dyslipidemia in little brown bats (Myotis lucifugus) and big brown bats (Eptesicus fuscus) with white nose syndrome**; Evan Pannkuk[1]; Nicole A. S.-Y. Dorville[2]; Yvonne A. Dzal[2]; Quinn E. Fletcher[2]; Kaleigh J.O. Norquay[2]; Craig K.R. Willis[2]; Albert J. Fornace Jr.[1]; Evagelia C. Laiakis[1]; [1]*Georgetown University Medical Center, Washington, DC; [2]University of Winnipeg, Winnipeg, MB*

MP 356 **Enhancement of lipid separation for the accurate quantification in nUHPLC-ESI-MS/MS**; Jong Cheol Lee[1]; Myeong Hee Moon[1]; [1]*Department of Chemistry, Yonsei University, Seoul, South Korea*

MP 357 **Analysis of lipogenesis kinetics and precursor pool enrichment by GC/MS-MIDA methodology for probing tissue-of-origin characteristics of plasma triglyceride-rich lipoproteins**; Sergiu P Palii[1]; Grace M Jones[1]; Angela C Arata[1]; Russell Caccavello[1]; Krishna K Barakoti[1]; Ewan F Sinclair[1]; Alejandro Gugliucci[1]; Jean-Marc Schwarz[1, 2]; [1]*Touro University California, Vallejo, CA; [2]University of California San Francisco, San Francisco, CA*

MP 358 **Investigation of the altered brain myelin lipidome in the neurodegenerative disorder, Niemann-Pick Type C1**; Chandimal Pathmasiri[1]; Melissa R. Pergande[1]; Fernando Tobias[2]; Stephanie M. Cologna[1]; Ernesto Bongarzone[1]; [1]*University of Illinois at Chicago, Chicago, IL; [2]The Ohio State University, Columbus, OH*

MP 359 **Evaluation of the viability of HILIC- and RP-LC-HRMS and lipidomics informatics for the characterization of strain-resolved Pseudomonas putida lipidomes**; David T. Reeves[1, 2]; William R. Henson[3]; Gregg T. Beckham[3]; Robert L. Hettich[1, 2]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee Knoxville, Knoxville, TN; [3]National Renewable Energy Laboratory, Golden, CO*

MP 360 **Elucidation of Lipid Markers Associated with Smoke Inhalation Injury Using Multidimensional Skyline Lipid Spectral Libraries**; Kaylie I Kirkwood[1]; Brian S. Pratt[2]; Kaipo Tamura[2]; Nicholas Shulman[2]; Sally Littau[3]; Amol M. Patwardhan[4]; Michael L. Heien[5]; Karen J. Richey[6]; Kevin N. Foster[6]; Jeffery L. Burgess[3]; Michael J. MacCoss[2]; Brendan X. Maclean[2]; Erin S. Baker[1]; [1]*Department of Chemistry, North Carolina State University, Raleigh, NC;*

[2]*Department of Genome Sciences, University of Washington, Seattle, WA; [3]Zuckerman College of Public Health, University of Arizona, Tuscon, AZ; [4]College of Medicine, University of Arizona, Tuscon, AZ; [5]Department of Chemistry and Biochemistry, University of Arizona, Tuscon, AZ; [6]The Arizona Burn Center, Maricopa Integrated Health Systems, Phoenix, AZ*

MP 361 **Role of neutral ceramidase in the pathogenesis of Alzheimer's Disease**; Farzana Parveen[1]; Vineet Kumar Mishra[1]; Shi Hui Law[1]; Hua-Chen Chan[2]; Liang-Yin Ke[1]; [1]*Kaohsiung Medical University, Kaohsiung City, Taiwan; [2]Kaohsiung Medical University Hospital, Kaohsiung, Taiwan*

MP 362 **Resolving the anti-ferroptotic role of Nitric Oxide: Inhibiting 15LO/PEBP1 complex-mediated phospholipid peroxidation**; Tamil Selvan Anthonymuthu[1]; Indira H Shrivastava[2]; Anastasia Levkina[3]; Georgiy Vladimirov[3]; Zachary E Hier[2]; Andrew Amoscato[2]; Valerian E. Kagan[2]; Hülya Bayır[2]; [1]*University Of pittsburgh, Pittsburgh, PA; [2]University of Pittsburgh, Pittsburgh, PA; [3]Laboratory of Navigational Redox Lipidomics, Institute of Regenerative Medicine, IM Sechenov Moscow State Medical University, Moscow,, Russia*

MP 363 **Spatially-resolved mass spectrometry approaches to study the role of lipid dysregulation in the pathogenesis of Glioblastoma**; Silvana Valdebenito[1]; Brendan Prideaux[2]; Eliseo Eugenin[2]; [1]*University of Texas Medical Branch, GALVESTON, TX; [2]University of Texas Medical Branch at Galveston, Galveston, TX*

MP 365 **A new method for the quantification of free fatty acids from disease state tissues**; Peter M Lococo[1]; Madeline Colley[2]; Kenneth M Hargreaves[3]; Stephen Bach[2]; [1]*UTHSCSA, San Antonio, TX; [2]University of Texas at San Antonio, San Antonio, TX; [3]UTHSCSA, San Antonio*

MP 366 **A Complete Solution for Lipidomic Profiling of Bladder Cancer Patients using a Compact LC-oa-TOF**; Lisa Reid[1]; Emmanuelle Claude[1]; Adam M King1; Gordon Fujimoto[2]; Robert Plumb[2]; Lauren Mullin[2]; [1]*Waters Corporation, Wilmslow, UK; [2]Waters Corporation, Milford, MA*

MP 367 **A Rapid HILIC-IM-MSE Method and Structure Database for Bacterial Lipidomics**; Christian Freeman[1]; Elijah Robert[1]; Kingsley Bimpeh[1]; Tabitha Lowe[1]; Shane Vahjen[1]; Keerthi Appala[1]; Kelly M Hines[1]; [1]*University of Georgia, Athens, GA*

MALDI: APPLICATIONS
MP 368-384

MP 368 **Lipidomic changes associated with ether lipid deficiency in germinal centers of spleen: A multimodal IMS approach**; Marissa Jones[1, 2]; Sung Hoon Cho[3]; Nathan Heath Patterson[1, 4]; Raf Van De Plas[5]; Clay F. Semenkovich[6, 7, 8]; Mark R. Boothby[3, 9, 10, 11, 12]; Jeffrey M. Spraggins[1, 2, 4]; Richard M. Caprioli[1, 2, 4, 9, 12]; [1]*Mass Spectrometry Research Center, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; [6]Division of Endocrinology, Metabolism & Lipid Research, Washington University School of Medicine, Saint Louis, MO; [7]Division of Biology and Biomedical Sciences, Washington University School of Medicine, Saint Louis, MO; [8]Department of Cell biology and Physiology, Washington University School of Medicine, Saint Louis, MO; [9]Department of Medicine, Vanderbilt University, Nashville, TN; [10]Department of Cancer Biology, Vanderbilt University, Nashville, TN; [11]Vanderbilt-Ingram Cancer Center, Vanderbilt University, Nashville, TN; [12]Department of Pharmacology, Vanderbilt University, Nashville, TN*

MP 369 **Multi-omic MS(/MS) analysis and identification of bacteria using liquid atmospheric pressure (AP) MALDI**; Sophie Lellman[1]; Rainer Cramer[1]; [1]*University of Reading, Reading, United Kingdom*

MP 370 **Development of a novel bio-detection method for discovery of disease-related molecules by the novel biochip, PepTenChip® in combination with MALDI-TOF-MS/MS**; Yuki Tominaga[1]; Takeshi Kasama[1]; Haruyuki Fujino[1]; Shun Nokihara[1]; Atsushi Kitagawa[1]; Kiyoshi Nokihara[1, 2]; [1]*HiPep Laboratories, Kyoto, Japan; [2]The First Affiliated Hospital with Nanjing Medical University, Nanjing, China*

MP 371 **Application of MALDI-MS for microcystin detection and imaging in mouse tissues**; Daria Kucheriavaia[1]; Nicholas J. Peraino[2]; Apurva Lad[1]; David J. Kennedy[1]; Steven T. Haller[1]; Judy A. Westrick[2]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH; [2]Wayne State University, Detroit, MI*

MP 372 **Comprehensive pigment identification in Chlorella vulgarisby intact chloroplast MALDI-ET analysis**; Luz A Calderón-Vergara[1]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza-Montañez[1]; [1]*Universidad Industrial de Santander, Santander, Colombia*

MP 373 **Novel High-Throughput MALDI-TOF MS Workflow for Screening of Different Analytes at Each Position on a Plate**; Sergei Dikler; *Bruker Scientific LLC, Billerica, MA*

MP 375 **Fabrication of Antibody Conjugated Gold Modified Aluminum Chip for the Selective Detection of Ketamine with MALDI-TOF MS Analysis**; Hsin-Ping Chen[1]; He-Hsuan Hsiao[1]; [1]*Department of Chemistry, National Chung Hsing University, Taichung city, Taiwan*

MP 376 **Fabrication of Antibody Decorated Boronic Acid Modified Gold Nanoparticles for the Rapid Diagnosis of Diabetes with LDI-TOF MS Analysis**; Li-Sin Tu[1]; He-Hsuan Hsiao[1]; [1]*Department of Chemistry, National Chung Hsing University, Taichung city, Taiwan*

MP 377 **Changes in thymosin β4 during enteroid generation demonstrated by direct MALDI-TOF-MS**; Mohan Acharya[1]; Rohana Liyanage[2]; Jackson O Lay Jr. [2]; Annie M Donoghue[3]; Narayan C Rath[3]; [1]*Department of Poultry Science , University of Arkansas, Fayetteville, Arkansas; [2]University of Arkansas, Fayetteville, AR; [3]USDA/Agricultural Research Service, Poultry Science Center, University of Arkansas, Fayetteville, Arkansas*

MP 378 **MALDI-MS mass spectrometry applied in the newborn screening for sickle cell disease: robustness, high throughput and cost-effectiveness**; Marven El Osta[1]; Pierre Naubourg[1]; Bichr Allaf[2]; Andreas Schnapp[3]; Tom K. Abban[4]; Shaukat Ibrahim[4]; Patrick Ducoroy[1]; [1]*Biomaneo, Dijon, France; [2]Hôpital universitaire Robert-debré, Paris, France; [3]Shimadzu Europa GmbH, Duisburg, Germany; [4]Shimadzu, Manchester, UK, Manchester, United Kingdom*

MP 379 **Metastable Decomposition at the Peptide C-Terminus-Possible Use in Protein Identification-**; Yang Wang[1, 2]; Etsuko Nakajima[1]; Yoshihito Okamura[1]; Danqing Wang[1, 3]; Nobuaki Okumura[1]; Toshifumi Takao[1]; [1]*Osaka University, Suita, Japan; [2]Cedars-Sinai Medical Center, Los Angeles, CA; [3]Fudan University, Shanghai, China*

MP 380 **High-Throughput Screening of Heavy Metal Ions with Peptide Decorated Gold Nanoparticles**; Tzu-Hui Chiang[1]; He-Hsuan Hsiao[1]; [1]*Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan*

MP 381 **Imaging mass spectrometry in the analysis of lipids and metabolites for pancreatic tumors**; Sina Feizbakhsh Bazargani[1]; Maria Guijarro Barrigon[2]; Richard A. Yost[2]; Maria Zajac-Kaye[2]; Timothy J. Garrett[2]; [1]*University of Florida, Gainesville, FL; [2]University of Florida, Gainesville*

MP 382 **Mass spectrometry signatures of rabbit VX2 carcinoma model using MALDI imaging**; Anna Colleen Crouch[1]; Dodge Lo Baluya[1, 2]; Emily A Thompson[1]; Elizabeth M Whitley[1]; Erik N.K. Cressman[1]; [1]*University of Texas MD Anderson Cancer Center, Houston, TX; [2]Washington State University, Pullman, WA*

MP 383 **Studying the selectivity of the interactions between G protein-coupled receptors and partner proteins by MALDI mass spectroscopy**; Na Wu[1]; Renato Zenobi[1]; Pikyee Ma[2]; [1]*ETH Zurich, Zurich, Switzerland; [2]Paul Scherrer Institute (PSI), Villigen, Switzerland*

MP 384 **Molecular Profiling of Neuropeptides in Lymnaea stagnalis by Matrix-Assisted Laser Desorption Ionization Mass Spectrometry with Heat Stabilization Treatment**; Ellen A. Wood[1]; Sara K. Mattson[1]; Sylwia Stopka[2]; Gabor Maasz[3]; Zsolt Pirger[3]; Akos Vertes[1]; [1]*Department of Chemistry, The George Washington University, Washington, DC; [2]Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [3]Department of Experimental Zoology, Balaton Limnological Institute, MTA Center for Ecological Research, Tihany, Hungary*

MALDI: FUNDAMENTALS AND INSTRUMENTATION
MP 385-388

MP 385 **Spatiotemporal distribution of neutral matrix molecules with high internal energy in the MALDI plume probed by VUV laser ionization**; Tatsuro Shirota[1]; Kennosuke Hoshina[1]; [1]*Niigata University of Pharmacy and Applied Life Sciences, Niigata, Japan*

MP 386 **Visual imaging studies of the N2 laser-generated plume in liquid atmospheric pressure (AP) matrix-assisted laser desorption/ionisation (MALDI)**; Evita Hartmane[1]; Henriette Krenkel[1]; Michael Morris[2]; Rainer Cramer[1]; [1]*University of Reading, Reading, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 387 **Disentangling distorted distributions - improving z' ion assignment confidence and structural characterization of proteins by top-down MALDI–in-source decay MS**; Simone Nicolardi[1]; David P. A. Kilgour[2]; Natasja Dolezal[3]; Jan W. Drijfhout[3]; Manfred Wuhrer[1]; Yuri E. M. Van Der Burgt[1]; [1]*Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands; [2]Department of Chemistry, Nottingham Trent University, Nottingham, United Kingdom; [3]Department of Immunohematology and Blood Transfusion, Leiden University Medical Center, Leiden, Netherlands*

MP 388 **Characterization of detection limits using sub-AP and AP MALDI sources utilizing high- and low-resolution mass spectrometers**; Eugene Moskovets[1]; Jace W. Jones[2]; Konstantin Novoselov[1]; Vladimir Doroshenko[1]; [1]*Mass Tech, Inc., Columbia, MD; [2]University of Maryland School of Pharmacy, Baltimore, MD*

MALDI: SAMPLE PREPARATION
MP 389-390

MP 389 **Hydrophilic/Hydrophobic Patterned Surfaces Fabricated by Laser Micromachining for Improved MALDI Sample Preparation**; Ben Tucker[1]; Matthias Hermann[1]; Haidy Metwally[1]; Richard Oleschuk[1]; [1]*Queen's University, Kingston, ON*

MP 390 **A simple device to ease, speed up, and standardise MALDI-TOF sample preparation**; Nadine Perrot[1]; Olivier Dauwalder[2]; Cécile Paris[3]; Alexia Barbry[2]; Stephanie Labich[3]; Corinne Beaulieu[3]; Bruno Colin[3]; Frederic Foucault[3]; Philippe Wandels[3]; Victoria Girard[1]; Karen Pinkston[4]; Geraldine Durand[1]; Francois Vandenesch[2]; Jean-Philippe

Charrier[3]; [1]BIOMERIEUX, La Balme Les Grottes, France; [2]Hospices Civils de Lyon (HCL), LYON, France; [3]BIOMERIEUX, Marcy L'etoile, France; [4]Biomerieux Inc, Hazelwood, MO 63042

METABOLOMICS: SAMPLE PREPARATION
MP 391-400

MP 391 **An Automated, Combined Workflow for Extracting Polar Metabolites and Lipids from Mammalian Cells**; Genevieve Van De Bittner[1]; Alex Apffel[1]; Thu T.A. Nguyen[2]; Kristin B. Bernick[1]; Manuel Gomez[1]; Dustin Chang[1]; Brian P. Smart[1]; Reid Brennen[1]; Christine Miller[1]; Steven Fischer[1]; Laurakay Bruhn[1]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*University of Illinois at Chicago, Chicago, IL*

MP 392 **Determining Minimum Cell Count for High-Quality Metabolite Identification and Metabolome Coverage**; Casey A. Chamberlain[1]; Kevin Cho[1]; Sarah Chiang[1]; Sisi Zhang[1]; Miriam Sindelar[1]; Steven R. Doonan[1]; Gary J. Patti[1]; [1]*Washington University in St. Louis, St. Louis, MO*

MP 393 **Nanosecond Photochemical Reaction (nsPCR) for Enhanced Identification and Visualization of Metabolites**; Yuan Liu[1]; Gongyu Li[1]; Lingjun Li[1, 2]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 394 **Automated Metabolomics Workflow of Dried Blood Spots Using a Novel Blood Microsampling Device**; Konstantinos A. Kouremenos[1, 2]; Robert Ninnis[1]; Christopher Bowen[2, 3]; David De Souza[4]; Kannan Ragunathan[1]; Wei Boon Hon[1]; Dedreia L. Tull[4]; Andrew A Gooley[1, 2]; [1]*Trajan Scientific and Medical, Melbourne, Australia;* [2]*Bio21 Institute, The University of Melbourne, Parkville, Australia;* [3]*Shimadzu Scientific Instruments, Rowville, Australia;* [4]*Metabolomics Australia, Bio21 Institute, The University of Melbourne, Parkville, Australia*

MP 395 **Cation exchange SPE utilized to remove alkali metal ions improves reproducibility and sensitivity for polar analytes in HILIC-ESI-MS analyses**; Ida Erngren[1]; Curt Pettersson[1]; Mikael Hedeland[1]; [1]*Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden*

MP 397 **Rapid analysis of S-Adenosylmethionine (SAM) and S-Adenosylhomocysteine (SAH) isotopologues in stable isotope-resolved metabolomics (SIRM) using direct nanoelectrospray ultra-high-resolution mass spectrometry**; Joonseon Yang[1]; Teresa Fan[1, 2, 3]; Andrew Lane[1, 2, 3]; Richard Higashi[1, 2, 3]; [1]*Center for Environmental & Systems Biochemistry, University of Kentucky, Lexington, KY;* [2]*Department of Toxicology and Cancer Biology, University of Kentucky, Lexington, KY;* [3]*Markey Cancer Center, University of Kentucky, Lexington, KY*

MP 398 **Evaluation of extraction methods for the simultaneous isolation of metabolites, lipids, and proteins for multi-omic analyses in Pseudomonas putida**; Matthew J Keller[1, 2]; David T Reeves[1, 2]; Richard J Giannone[1]; Robert L Hettich[1]; [1]*Oak Ridge National Laboratory (ORNL), Oak Ridge, TN;* [2]*University of Tennessee, Knoxville, TN*

MP 399 **Assessment of a Metabolomics Automated Sample Prep Platform for Low Volume Plasma Samples**; Mark Sartain[1]; Manuel Gomez[1]; Genevieve Van De Bittner[1]; Henry Shu[1]; [1]*Agilent Technologies, Santa Clara, CA*

MP 400 **Impact of microcentrifuge tube selectionon metabolomic results and some suggestions for best practices**; Ah Young Yoon[1]; Sujatha Chilakala[1]; Stella Somiari[2]; Katie Miller[2]; Heather Blackburn[2]; Vijay Eedunuri[2]; Hai Hu[2]; Jerry S.H. Lee[1, 3]; Jonathan E Katz[1]; [1]*Lawrence J. Ellison Institute for Transformative Medicine of USC, LOS ANGELES, CA;* [2]*Chan Soon-Shiong Institute of Molecular Medicine at Windber, Windber, Pennsylvania;* [3]*Department of Medicine/Oncology, Keck School of Medicine, Department of Chemical Engineering and Material Sciences, Viterbi School of Engineering, University of Southern California, Los Angeles, California*

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS
MP 401-425

MP 401 **Fast and Sensitive determination of Targeted Intracellular Metabolites in Biological Fluids Using HILIC Negative Electrospray-Mass Spectrometry**; Liangqiao Bian[1]; Chongshan Dai[2]; Ruiliu Wu[2]; Rui Kang[2]; Daolin Tang[2]; [1]*Shimadzu Center for advanced analytical chemistry, Arlington, Texas;* [2]*Department of Surgery, University of Texas Southwestern medical center, Dallas, Texas*

MP 402 **Simultaneously quantitative profiling of 18 bile acids in human gastrointestinal fluid by a rapid UPLC-MS/MS assay**; Ruiting Li[1]; Bo Wen[1]; Praveen Kumar[1]; Jeremy Felton[1]; Amit Pai[1]; Duxin Sun[1]; [1]*University of Michiagan, Ann Arbor, MI*

MP 403 **Quantitative analysis of acylcarnitines including isomeric and isobaric forms in biological matrices**; Maheshwor Thapa[1, 2]; Daniela D. Weber[1]; Sepedeh Aminzadeh Gohari[1]; Barbara Ustaszewski[2]; Barbara Kofler[1]; Guido Dallmann[2]; Therese Koal[2]; [1]*Research Program for Receptor Biochemistry and Tumor Metabolism, Department of Pediatrics, Paracelsus Medical University, Salzburg, Austria;* [2]*BIOCRATES Life Sciences AG, Innsbruck, Austria*

MP 404 **A fast and robust LC-DMS-MRMHR method to increase isobar separation power for tracking isotope labels in central carbon metabolism**; Qiushi Sun[1]; Richard Williams[1]; Richard G. Kibbey[1]; [1]*Yale University, New Haven, CT*

MP 405 **Using LC-MS/MS to understand peripheral amino acid changes in Obesity and Alzheimer's Disease**; Amelia L. Taylor[1]; Simona G. Codreanu[1]; Don E. Davis, Jr. [1]; Christina C. Marasco[1]; Fiona E. Harrison[2]; Stacy D.

Sherrod[1]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Vanderbilt University Medical Center, Nashville, TN*

MP 406 **Targeted Metabolite Quantitation by MRM in Cell Culture Media: Evaluating Methods to Streamline Metabolite Analysis to Guide Cell Line Development**; Elsa Gorre[1]; Andrew D Mahan[2]; [1]*JOHNSON AND JOHNSON, Spring House, PA;* [2]*Johnson and Johnson, Spring House, PA*

MP 407 **Development of polar metabolite profiling method by supercritical fluid chromatography/tandem mass spectrometry**; Yutaka Konya[1]; Yoshihiro Izumi[2]; Takeshi Bamba[1]; [1]*Kyushu University, Fukuoka, Japan;* [2]*Kyushu University, Fukuoka, Japan*

MP 408 **Quantification of Metabolites Using the UPLC/MS-based AbsoluteIDQ p180 Kit**; Vasanta Putluri[1]; Arun Sreekumar[1]; Nagireddy Putluri[1]; [1]*Baylor College of Medicine, Houston, TX*

MP 409 **Integrating metabolomics as an important tool in pharmaceutical and biopharmaceutical drug research, discovery and development: Application case studies**; Dewakar Sangaraju[1]; Allan Jaochico[1]; Zijuan Lai[1]; Meryssa Tran[1]; Xiaorong Liang[1]; Nadja Katheder[1]; Heinrich Jasper[1]; Mary Keir[1]; Jordan Mar[1]; Allyson Byrd[1]; Jonathan Maher[1]; Tanja Zabka[1]; Paula Katavolos[1]; Anh Nguyen Dang[1]; Robert Shawley[1]; Yao Shi[2]; Clay Williams[2]; Dennis Milanowski[2]; Rachel Caminiti[2]; [1]*Genentech Inc, South San Francisco, CA;* [2]*Covance Laboratories Inc., Madison, WI*

MP 410 **A rapid and high throughput method for LC-MS/MS based quantification of indol-3-acetic acid and trans-Zeatin**; Anish Kundu[1, 2]; Khushboo Adlakha[1, 2]; Divya Goyal[1]; Faraz Rashid[2]; Dipankar Malakar[2]; Jyothilakshmi Vadassery[1]; [1]*National Institute of Plant Genome Research, Aruna Asaf Ali Marg,, New Delhi, India;* [2]*SCIEX, 121,Udyog Vihar, Phase – IV, Gurgaon, Haryana, India*

MP 411 **Ovarian Cancer Metabolomics: Targeted Microchip Capillary Electrophoresis-Mass Spectrometry to Track Disease Progression**; Samyukta Sah[1]; Marcos Bouza Areces[2]; Eunyong Park[3]; Olga Kim[3]; Jaeyeon Kim[3, 4]; Facundo Fernández[2]; [1]*Georgia Tech, Atlanta, GA;* [2]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia;* [3]*Indiana University School of Medicine, Departments of Surgery, Biochemistry and Molecular Biology, Indianapolis, Indiana;* [4]*Indiana University Melvin & Bren Simon Cancer Center, Indianapolis, IN*

MP 412 **Quantitation of amino sugars in leaf litter by chemical derivatization - LC/MS**; Jun Han[1, 2]; Alexandra Klem[3]; Evan Dyson-Loewen[1]; Juncong Yang[1]; David Schibli[1]; David R. Goodlett[4, 5]; [1]*University of Victoria - Genome BC Proteomics Centre, Victoria, BC;* [2]*Division of Medical Sciences, University of Victoria, Victoria, BC;* [3]*University of Waterloo, Waterloo, ON;* [4]*University of Maryland School of Dentistry, Baltimore, MD;* [5]*University of Gdansk, International Centre for Cancer Vaccine Science, Gdsnsk, Poland*

MP 413 **Potential of metabolite sums and ratios calculations for faster biological insights into targeted metabolomics data**; Martin Buratti[1]; Barbara Ustaszewski[1]; Gordian Adam[1]; Fadi Abdi[1]; Therese Koal[1]; [1]*BIOCRATES Life Sciences AG, Innsbruck, Austria*

MP 414 **Wide-range metabolomic analysis of hydrophilic metabolites by next-generation ion chromatography high resolution tandem mass spectrometry**; Masatomo Takahashi[1]; Yoshihiro Izumi[1]; Takahiro Suzuki[2]; Kohta Nakatani[1]; Kosuke Hata[1]; Kentaro Takahara[2]; Takeshi Bamba[1]; [1]*Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan;* [2]*Thermo Fisher Scientific, Yokohama, Japan*

MP 415 **Derivatization Approaches for Endogenous Steroid Hormones in Human Urine Using High-Resolution LC-MS**; Lancia N.F. Darville-Bowleg[1]; Jayden C Cline[1]; Carrie Rozmeski[1]; Yessica C Martinez[1]; Shannan Rich[2]; Kathleen M Egan[1]; Lusine Yaghjyan[2]; John M Koomen[1]; [1]*Moffitt Cancer Center, Tampa, FL;* [2]*University of Florida, Gainesville, FL*

MP 416 **Measurement of methylated metabolites using liquid chromatography-mass spectrometry**; Chandra Shekar R Ambati[1]; Nagireddy Putluri[1, 2]; Arun Sreekumar[3]; [1]*Advanced Technology Core, Dan L. Duncan Cancer Center, Alkek Center for Molecular Discovery, Baylor College of Medicine, Houston, TX 77030;* [2]*Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX 77030;* [3]*Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX, USA, Houston, TX 77030*

MP 417 **Screening and Quantitation of Amino Acid and other components in Spent Media**; Vikrant Goel[1]; Ashish Pargaonkar[2]; Sunil Raut[3]; Swarnendu Kaviraj[3]; Saikat Banerjee[4]; [1]*Agilent Technologies, Gurgaon, India;* [2]*Agilent Technologies, BENGALURU, India;* [3]*Gennova Biopharmaceuticals Ltd, Pune, India;* [4]*Agilent Technologies India Pvt Ltd, Hyderabad, India*

MP 418 **SCIEX 6500+ ESI-MS/MS: Impact of Advanced Scanning sMRM Mode on Peak Quality in Broad-spectrum metabolomics**; Atul S Rathore[1]; Preeti Chandra[1]; Monique C Santana[1]; Colin D Kay[1]; [1]*Food Bioprocessing & Nutrition Sciences, Plants for Human Health Institute, North Carolina State University, North Carolina Research Campus, 600 Laureate Way, Kannapolis, NC*

MP 419 **Targeted metabolic analysis of tricarboxylic acid cycle intermediates and amino acids in human plasma following chemical derivatization**; Adam Cseresznye[1, 2]; Claire Jeanine Colette Huguenard[1, 2, 3]; James E. Evans[1, 2]; Michael Mullan[1, 2, 4]; Fiona Crawford[1, 2, 4]; Laila Abdullah[1, 2, 4]; [1]*Roskamp Institute, Sarasota, FL;*

[2]*James A. Haley Veterans' Hospital, Tampa, FL;* [3]*Open University, Milton Keynes, United Kingdom;* [4]*Open University, Milton Keynes, United Kingdom*

MP 420   **Laser Ablation Electrospray Ionisation Mass Spectrometry (LAESI-MS) analysis of terpenoids for biotechnology applications**; Andres Galindo Garcia; *The University of Manchester, Manchester, United Kingdom*

MP 421   **Widely targeted metabolomics of hydrophilic compounds in wine using two LC-MS/MS methods: Comparison of different types and producing regions**; Yasuko Yamada[1]; Takanari Hattori[2]; Jun Watanabe[2]; Junko Iida[2]; [1]*Shimadzu Techno-Research, Inc., Kyoto, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan*

MP 422   **Multiplexed quantification of bile acids with LC-MS for characterization of mouse gut microbial metabolism**; Armando Alcazar Magana[1, 2]; Yang Zhang[2, 3]; Adrian Gombart[2, 4]; Jan F. Stevens[2, 5]; Claudia Susanne Maier[1, 2]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*Linus Pauling Institute, Corvallis, Oregon;* [3]*School of Biological and Population Health Sciences, Corvallis, Oregon;* [4]*Department of Biochemistry and Biophysics, Oregon State University, Corvallis, Oregon;* [5]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, Oregon*

MP 423   **Development of cell culture supernatant analysis using LC-MS/MS and their application for Chinese hamster ovary cell**; Kenichi Toyoda[1]; Hirotaka Kuroda[1]; Takashi Suzuki[1]; Toru Ezure[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

MP 424   **Contribution of host arginine metabolism to malaria infection outcomes – HILIC based LC-MS/MS analysis of free amino acids**; Karolina M. Krasinska[1]; Nicole M. Davis[2]; Zijie Xia[1]; David S. Schneider[2]; Allis S. Chien[1]; [1]*Stanford University Mass Spectrometry, Stanford, CA;* [2]*Dept. of Microbiology & Immunology, Stanford University, Stanford, CA*

MP 425   **Absolute quantification of abemaciclib in murine plasma and amniotic fluid using matrix-controlled standard curve with solid phase extraction and LC-MS/MS**; Yik Siu[1]; Daniele Simoneschi[1]; Michele Pagano[1]; Drew Jones[1]; [1]*NYU Langone Health, New York, NY*

MICROORGANISMS AND THE MICROBIOME I
MP 426-441

MP 426   **Accounting for chimeric spectra boosts the number of identifications in metaproteomics without impacting sensitivity**; Tim Van Den Bossche[1]; Thilo Muth[2]; Lennart Martens[1]; Viktoria Dorfer[3]; [1]*VIB - UGent Center for Medical Biotechnology, Gent, Belgium;* [2]*eScience Division (S.3), Federal Institute for Materials Research and Testing, Berlin, Germany;* [3]*Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria*

MP 427   **Visualizing mineral cation uptake in fungal hyphae and elucidating the resulting changes in the proteome**; Arunima Bhattacharjee[1]; Odeta Qafoku[1]; Kaitlyn Schwarz[1]; Zihua Zhu[1]; Lindsey Anderson[1]; Geremy Clair[1]; William Nelson[1]; Mark Engelhard[1]; Mark Bowden[1]; Janet Jansson[1]; Kirsten Hofmockel[1]; Christopher Anderton[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

MP 428   **Mass spectrometry-based metaproteomics study of microbiome-host interactions in 5/6 nephrectomy mouse model of Chronic Kidney Disease during dietary fiber supplementation**; Oleg Karaduta[1]; Zeljko Dvanajscak[2]; Galina Glazko[1]; Yasir Rahmatallah[1]; Alan Tackett[1]; Lisa Orr[1]; Samuel Mackintosh[1]; John Arthur[1]; Boris Zybaylov[1]; [1]*UAMS, Little Rock, AR;* [2]*Arkana Laboratories, Little Rock, AR*

MP 429   **Analysis of fecal metabolome to study the function of Microbiota in rats with neuropathic pain treated by Ginger root extract**; Masoud Zabet Moghaddam[1]; Xiaoxia Gong[2]; Parvin Mirzaei[2]; Rui Wang[3]; Volker Neugebauer[3]; Yehia Mechref[2]; Chwani-Li Shen[3]; [1]*Texas Tech University, Box 43132 Lubbock, TX;* [2]*Texas Tech University, Lubbock, Texas;* [3]*Texas Tech University Health Sciences Center, lubbock,, TX*

MP 430   **Identification of clinically relevant microbes directly from culture and infected tissues with the MasSpec Pen**; Sydney C Povilaitis[1]; Ashish Chakraborty[1]; Lindsey Kirkpatrick[2]; Rachel D Downey[3]; Sarmistha B Hauger[3, 4]; Livia S Eberlin[1]; [1]*University of Texas Austin, Austin, TX;* [2]*Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN;* [3]*Dell Children's Medical Center, Austin, TX;* [4]*Dell Medical School, Austin, TX*

MP 431   **The Metabolic State Of Syntrophic Bacteria Effects Proteomic Acylation Profile**; John Muroski[1]; Hong H Nguyen[1]; Michael J McInerney[2]; Rachel RO Loo[1]; Joseph A. Loo[1]; [1]*University of California, Los Angeles, Los Angeles, CA;* [2]*University of Oklahoma, Norman, OK*

MP 432   **Host diet directs structure and immunomodulatory capacity of gut symbiont-originated glycosphingolipids**; Sungwhan F Oh[1, 2]; Jisun Yoo[1]; Changwon C Lee[2]; Deniz Erturk-Hasdemir[2]; Hee Bum Song[3]; Ledia Gebremedhin[1]; Seung Bum Park[3]; Dennis L Kasper[2]; [1]*Brigham and Women's Hospital, Boston, MA;* [2]*Harvard Medical School, Boston, MA;* [3]*Seoul National University, Seoul, South Korea*

MP 433   **The rhizosphere signature on the cell motility, biofilm formation and secondarymetabolite production of a plant-associated Lysobacter strain**; Francesca Brescia[1, 2]; Ilaria Pertot[1, 3]; Gerardo Puopolo[1]; Martina Marchetti-Deschmann[4]; [1]*Fondazione Edmund Mach, San Michele all'Adige, Italy;* [2]*University of Udine, Udine, Italy;* [3]*University of Trento, San Michele all'Adige, Italy;* [4]*TU Wien, Vienna, Austria*

MP 434 **Predicting metabolite production in gut microbes by integrating flux balance analysis with untargeted metabolomics**; Erica Marie Forsberg[1]; Matt Marney[1]; Ellen Kuang[1]; Rob Edwards[1]; [1]*San Diego State University, San Diego, CA*

MP 435 **Proteolytic Maturation and Copy Number Determination in a Giant SalmonellaVirus**; Aaron Scheuch[1]; Sara Mallory[1]; Julia Faraone[1]; Sammy Pardo[2]; Dana Molleur[3]; Ru-ching Hsia[4]; Susan T. Weintraub[3]; Julie A. Thomas[1]; [1]*Rochester Institute of Technology, Rochester, NY 14623-5603; [2]University of Texas Health Science Center at San Antonio, San Antonio, TX 78229-3900; [3]University of Texas Health Science Center at San Antonio, San Antonio, TX 78229; [4]University of Maryland School of Dentistry, Baltimore, MD 21201*

MP 436 **Morphine administration, genetics, and high fat diet alters the mouse gut microbiome composition and function in lean and obese mice**; Jose Alfredo Blakeley-Ruiz[1, 2]; Carlee S. Mcclintock[2, 3]; Him K Shrestha[1, 2]; Suresh Poudel[2]; Richard J. Giannone[2]; Mircea Podar[1, 2]; Helen A. Baghdoyan[1, 2]; Ralph Lydic[2, 4]; Robert L. Hettich[1, 2]; [1]*University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; [3]Pain Consultants of East Tennessee, Knoxville, TN; [4]University of Tennessee Knoxville, Knoxville, TN*

MP 437 **Proteomic and metabolomic characterization of the syntrophic interactions between TM7 phylotype and Actinomyces odontolyticus**; Fabian Schulte[1, 2]; Batileg Bor[1, 2]; Lujia Cen[1]; Pooja Balani[1, 2]; Tsute Chen[1]; Markus Hardt[1, 2]; Xuesong He[1, 2]; [1]*Forsyth Institute, Cambridge, MA; [2]Harvard School of Dental Medicine, Boston, MA*

MP 438 **MiCldGUI: A user friendly graphical interface for MiCld a tool for Microorganism Classification and Identification**; Aleksey Ogurtsov[1]; Gelio Alves[1]; Yi-Kuo Yu[1]; [1]*National Center for Biotechnology Information, NLM, Bethesda, MD*

MP 439 **LC-HRMS and GCxGC-TOFMS characterization of storage conditions for metabolite screening in human whole stool samples**; Paulina Piotrowski[1]; Christina Jones[2]; [1]*National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, Maryland*

MP 440 **A practical workflow for training in gut metaproteomics studies**; Mona M. Khamis[1]; Xu Zhang[1]; Zhibin Ning[1]; Krystal Walker[1]; Leyuan Li[1]; Kai Cheng[1]; Janice Mayne[1]; Daniel Figeys[1]; [1]*Ottawa Institute of Systems Biology and Department of Biochemistry, Microbiology and Immunology, University of Ottawa, Ottawa, ON*

MP 441 **The Archaeal Proteome Project – advancing knowledge about archaeal cell biology through comprehensive proteomics**; Stefan Schulze[1]; Zachary Adams[2]; Micaela Cerletti[3]; Rosana De Castro[3]; Sébastien Ferreira-Cerca[4]; Christian Fufezan[5]; María Inés Giménez[3]; Michael Hippler[6]; Zivojin Jevtic[7]; Robert Knüppel[4]; Georgio Legerme[2]; Christof Lenz[7]; Anita Marchfelder[8]; Julie Maupin-Furlow[2]; Roberto A. Paggi[3]; Friedhelm Pfeiffer[7]; Ansgar Poetsch[9]; Henning Urlaub[7]; Mechthild Pohlschroder[1]; [1]*University of Pennsylvania, Philadelphia, PA; [2]University of Florida, Gainesville, FL; [3]National University of Mar del Plata, Mar del Plata, Argentina; [4]University of Regensburg, Regensburg, Germany; [5]Heidelberg University, Heidelberg, Germany; [6]University of Münster, Münster, Germany; [7]Max Planck Institute for biophysical chemistry, Göttingen, Germany; [8]Ulm University, Ulm, Germany; [9]Ruhr University Bochum, Bochum, Germany*

MP 442 **Liver Toxicity and Alteration of Renin-Angiotensin System (RAS) Components Induced by Silver Nanoparticle Exposure in Wistar Rats**; Subhayu Nayek[1]; Imesha W. De Silva[1]; Amie K. Lund[1]; Guido F. Verbeck[1]; [1]*University of North Texas, Denton, TX*

NANOMATERIALS
MP 442-445

MP 443 **Characterization of Nanoparticles Embedded in Organic Matrices by Cluster-SIMS**; Stanislav Verkhoturov[1]; Nathan A. Fleer[2]; Dmitriy S. Verkhoturov[2]; Guan-Wen Liu[2]; Michael J. Eller[2]; Sarbajit Banerjee[1]; Emile A. A. Schweikert[2]; [1]*Texas A&M University, College Station, TX; [2]Texas A&M, College Station, TX*

MP 444 **Structure and dynamics of inorganic polymers in solution studied with high-resolution MS, LC/MS and 16O/18O exchange: focus on polyoxometales**; Daniel Favre[1]; Igor A Kaltashov[1]; [1]*Univ. of Massachusetts/Chemistry Dept., Amherst, MA*

MP 445 **Quantitative LC-MS/MS Analysis of PEGylated and non-PEGylated Lipid Mixtures from Lanthanide Nanoparticle-Supported Lipid Bilayers**; Loryn P. Arnett[1]; Matthew W Forbes[1]; Mitchell A. Winnik[1]; [1]*University of Toronto, Toronto, ON*

NATURAL PRODUCTS
MP 446-453

MP 446 **Separation and detection method for polyphenols and its associated isomers using ion-mobility mass spectrometry**; Iwao Sakane[1]; Hajime Mizuno[2]; Eiji Sugiyama[2]; Kentaro Takahara[3]; Reiko Kiyonami[4]; [1]*ITO-EN LTD, Tokyo, Japan; [2]University of Shizuoka, Shizuoka, Japan; [3]Thermo Fisher Scientific Japan, Tokyo, Japan; [4]Thermo Fisher Scientific, San Jose, CA*

MP 447 **Analysis ofVitamin E acetate in Hemp vape oil products**; <u>Sue Dantonio</u>[1]; Robert A. Dantonio[2]; Nikolas Lau[3]; [1]*Agilent Technologies, Cedar Creek, TX;* [2]*Texas A & M University, Corpus Christi, Texas;* [3]*Agilent Technologies, Chicago, IL*

MP 448 **Structural moieties and tissue distribution of hepatoprotective lignin-derived agent determined by isotopic labeling mass spectrometry**; <u>Alexander Zherebker</u>[1]; Oleg Kharybin[1]; Alexey Orlov; Oxana Kovaleva[1]; Oliver J. Lechtenfeld[2]; Elena Fedoros[3]; Irina Perminova[4]; Eugene (evgeny) Nikolaev[5]; [1]*Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation;* [2]*Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany;* [3]*N.N. Petrov National Medical Research Center of Oncology, Saint-Petersburg, Russia;* [4]*Lomonosov Moscow State University, Chemistry Department, Moscow, Russia;* [5]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 449 **Discovery of Bioactive Proteins from Scorpion Venom using Two Dimensional Mass Spectrometry**; <u>Meng Li</u>[1]; Yuko Pui Yiu Lam[1]; Christopher A. Wootton[1]; Peng Chen[2]; Remy Gavard[1]; Cookson K. C. Chiu[1]; Bryan P. Marzullo[1]; Qiong Wu[2]; Tomos E. Morgan[1]; Mark P. Barrow[1]; Hongzheng Fu[2]; Peter B O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*Peking University, Haidian, China*

MP 450 **Cyclic Peptide Tandem-MS Search Software**; Marshall Bern[1]; <u>A. Michelle English</u>[1]; Wilfred Tang[1]; Chia-Wei Chia-Wei Lin[2]; Hannelore Kaspar[2]; Emmanuel Matabaro[2]; Markus Künzler[2]; [1]*Protein Metrics, Cupertino, CA;* [2]*ETH Zurich, Zurich, Switzerland*

MP 451 **Establishment and application of a natural product LC-MS/MS library for plant metabolomics**; <u>Wenbin Wu</u>[1]; Jeffrey Morré[2]; Valtcho Jeliazkov[3]; Jett Guerra[4]; Jan F. Stevens[1]; [1]*Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon 97331;* [2]*Department of Chemistry, Oregon State University, Corvallis, Oregon 97331;* [3]*Department of crop and soil science, Oregon state university, Corvallis, Oregon 97331;* [4]*Department of Botany and Plant Pathology, Oregon State University, Corvallis, Oregon 97331*

MP 452 **Advancing the Throughput and Sensitivity of Magnetic Microbead Affinity Selection-Mass Spectrometry (MagMASS) for Natural Products Drug Discovery**; <u>Richard B. Van Breemen</u>[1]; Ruth N. Muchiri[1]; Jaewoo Choi[2]; Dana M. Gibbon[1]; Brett Tyler[1]; [1]*Oregon State University, Corvallis, OR;* [2]*Oregon State Univeristy, Covallis, Oregon*

MP 453 **Effects of Sample Preparation Method on Metabolomic and Bioactivity Profiles of Mango (Mangifera indica) Extracts: A Feature-Based Molecular Networking Approach**; Cesar P. Quizon[1]; <u>Michael Russelle S. Alvarez</u>[1]; Kimberly M. Delica[1]; Manolo L. Basingan, Jr[1]; Froila Marie G. Deniega[1]; Rowell P. Abogado[2]; Patrick Moreno[3]; Luster S. Labarga[1]; Mylene Ross P. Arcena[1]; Isagani D. Padolina[2]; Francisco M. Heralde Iii[3]; Gladys Cherisse J. Completo[1]; Ruel C. Nacario[1]; [1]*University of the Philippines Los Baños, Laguna, Philippines;* [2]*Pascual Pharma Corp., Laguna, Philippines;* [3]*Lung Center of the Philippines, Quezon City, Philippines*

PEPTIDES: PTM IDENTIFICATION I
MP 454-468

MP 454 **Multi-Level Post-Translational Modification Classification with PTM-Shepherd**; <u>Daniel J Geiszler</u>[1]; Dmitry Avtonomov[1]; Andy Kong[1]; Fengchao Yu[1]; Felipe V Leprevost[1]; Hui-Yin Chang[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 455 **Mass spectrometry-based precise identification of endogenous citrullinated histone in human astrocytoma U87 cells**; <u>Bin Wang</u>[1]; Yatao Shi[1]; Zihui Li[2]; Xudong Shi[3]; Lingjun Li[1, 2]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706;* [3]*Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI 53705*

MP 456 **Stoichiometric quantification of protein persulfidation in response to stress conditions**; <u>Xiaolu Li</u>[1, 2]; Tong Zhang[1]; Matthew J. Gaffrey[1]; Ronald J. Moore[1]; Bin Yang[2]; Wei-Jun Qian[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Washington State University, Richland, WA*

MP 457 **Disulfide bond and glycosylation site occupancy mapping of monoclonal antibodies using a novel capillary MAbPac column**; <u>Zoltan Szabo</u>[1]; Xuefei Sun[2]; Brandon H. Robson[2]; Lin Shanhua[2]; Dietmar Reusch[3]; Mike Baynham[4]; Rainer Bauder[5]; [1]*Thermo Fisher Scientific, Sunnyvale, CA;* [2]*Thermo Fisher Scientific, Sunnyvale, California;* [3]*Roche Diagnostics GmbH, Penzberg, Germany;* [4]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [5]*Thermo Fisher Scientific, Chelmsford, MA*

MP 458 **Fragmentation of insulin and related compounds by electron capture dissociation in a modified quadrupole-time of flight mass spectrometer**; <u>Michael C Hare</u>[1]; Valery G. Voinov[1, 2]; Yury V. Vasil'ev[1, 2]; Joseph C. Meeuwsen[1, 2]; Joseph S. Beckman[1, 2]; [1]*e-MSion Inc., Corvallis, Oregon;* [2]*Oregon State University, Corvallis, OR*

MP 459 **Characterization of Capsid Protein Post Translational Modifications Using High Resolution Mass Spectrometry**; <u>Sean Mccarthy</u>[1]; Kerstin Pohl[2]; Esme Candish[2]; [1]*SCIEX, Framingham, MA;* [2]*Sciex, Framingham, MA*

MP 460 **MS Characterization of Extensin Peptides From Cell Walls: Identification of Intra- and Intermolecular Cross-links and Abundance of Internal Fragment Ions**; <u>Lawrie Veale</u>[1]; Ankur Patel[2]; Steven D Hartson[1];

Michelle English[3]; Marshall Bern[3]; Andrew J Mort[1]; [1]*Oklahoma State University, Stillwater, OK;* [2]*University of Sheffield, Sheffield, United Kingdom;* [3]*Protein Metrics Inc, Cupertino, CA*

MP 461 **Counterion Optimization Dramatically Improves Selectivity for Phosphopeptides and Glycopeptides in Electrostatic Repulsion-Hydrophilic Interaction Chromatography (ERLIC)**; <u>Yusi Cui</u>[1]; Dylan Nicholas T Tabang[1]; Zishan Zhang[1]; Min Ma[1]; Andrew J. Alpert[1, 2]; Lingjun Li[1]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*PolyLC Inc., Columbia, MD*

MP 462 **Revealing dynamic protein acetylation across subcellular compartments**; <u>Alexis J Lawton</u>[1]; Josue Baeza[1]; John Denu[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin*

MP 463 **Development of a novel mass spectrometry decision tree for O-GlcNAc site mapping**; <u>John W. Thompson</u>[1]; Michael J. Sweredoski[2]; Matthew E. Griffin[1]; Brett Lomenick[2]; Annie Moradian[2]; Spiros D. Garbis[2]; Linda C. Hsieh-Wilson[1]; [1]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125;* [2]*Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA 91125*

MP 464 **A Rapid Analysis of Enantiomers and Isomers of Aspartyl Residues in Proteins by Targeted Proteomics Approach using Micro-flow LC-MS/MS**; Noriko Fujii[1]; Takumi Takata[1]; Ingu Kim[1]; <u>Toshiya Matsubara</u>[2]; [1]*Institute for Integrated Radiation and Nuclear Science, Kyoto University, Sennan-gun, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan*

MP 465 **Complementarity of EThcD and HCD of Glycopeptides: Y ion Filtering for Increased Glycopeptide Identification**; <u>Robert Chalkley</u>[1]; Katalin F Medzihradszky[1, 2]; Adam Pap[2]; Zsuzsanna Darula[2]; Peter R Baker[1]; [1]*University of California San Francisco, San Francisco, CA;* [2]*Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary*

MP 466 **Proteogenomics meta analysis for unraveling the sources of MHC class I neoantigens in cancer**; <u>Georges Bedran</u>[1]; Marcos Yebenes[1]; Sachin Kote[1]; Irena Dapic[1]; Kamila Pawlicka[2]; Satya Saxena[3]; David Goodlett[4]; Robin Fahraeus[1, 5]; Ted Hupp[1, 2]; Javier A Alfaro[1, 2]; [1]*University of Gdansk, International Centre for Cancer Vaccine Science, Gdsnsk, Poland;* [2]*University of Edinburgh, Edinburgh, United Kingdom;* [3]*Deurion LLC, Seattle, WA;* [4]*University of Maryland Balitmore, Baltimore, MD;* [5]*INSERM, Paris, France*

MP 467 **Mass spectrometric quantification of histone lactylation marks in human melanoma cells**; Kevin Huang[1, 2]; Ziyuan Li[1, 3]; Lu Yang[1]; Jinjun Gao[1]; <u>Di Zhang</u>[1]; Yingming Zhao[1]; [1]*Ben May Department for Cancer Research, The University of Chicago, Chicago, Illinois;* [2]*St. Mark's School in Southborough, Massachusetts, MA;* [3]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 468 **Polyubiquitin chain architecture detected by mass spectrometry**; <u>bo-shieng Hsu</u>; *National Taiwan Ocean University, Keelung, Taiwan*

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS
MP 469-495

MP 469 **Characterization of the nucleoprotein complex Redβ by native mass spectrometry**; <u>Andrew Norris</u>[1]; Brian Caldwell[1]; Charles Bell[1]; Vicki H. Wysocki[1]; [1]*The Ohio State University, Columbus, OH*

MP 470 **Collision Induced Dissociation of Higher-Order Hemoglobin Complexes Reveals Quaternary Structure Information**; <u>Alexander I.M. Sever</u>[1]; Victor Yin[1]; Lars Konermann[1]; [1]*The University of Western Ontario, London, ON*

MP 471 **Application of Protein Folding and Stability Measurements to the Analysis of Protein-Metal Interactions on the Proteomic Scale**; <u>Nancy Wiebelhaus</u>[1]; Jacqueline M. Zaengle-Barone[1]; Katherine J. Franz[1]; Michael C. Fitzgerald[1]; [1]*Duke University, Durham, NC*

MP 472 **Differential assembly of ERBB signaling complex provides mechanistic insight on kinase inhibitor sensitivity in cancer cells**; <u>Shujuan Wang</u>[1]; Cunjie Zhang[2]; Xiaojing Wu[1]; Pan Zhang[1]; Qing Sheng[3]; Carl Uli Bialucha[3, 4]; Karen Colwill[4]; Yong Zheng[1]; [1]*Beijing Proteome Research Center,National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China;* [2]*Lunenfeld Tanenbaum Research Institute, Toronto, M5G 1X5;* [3]*Novartis Institutes for Biomedical Research, Cambridge, Massachusetts;* [4]*Lunenfeld Tanenbaum Research Institute, Mount Sinai Hospital, Toronto, M5G 1X5*

MP 473 **Native mass spectrometry analysis of the macromolecular organization of Get3-Get4-Get5 protein complex**; <u>Fabian Giska</u>[1]; Malaiyalam Mariappan[1]; Kallol Gupta[1]; [1]*Nanobiology Institute, Department of Cell Biology, Yale School of Medicine, West Haven, CT*

MP 474 **Probing the interaction of liver fatty acid binding protein and bezafibrate by native liquid extraction surface analysis mass spectrometry**; <u>Eva Illes-Toth</u>[1]; James W. Hughes[1]; Helen J. Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

MP 475 **How variable is your pore-forming protein toxin oligomeric state in different detergent environments?**; <u>Amber D. Rolland</u>[1]; Jesse W. Wilson[1]; Lejla S. Biberic[1]; James S. Prell[1]; [1]*University of Oregon, Eugene, OR*

MP 476 **Check before you plunge: native MS as a diagnostic and screening platform in preparing macromolecular assemblies for cryo-EM analysis**; Paul Dominic B. Olinares[1]; James Chen[1]; Courtney Chiu[1]; Jin Young Kang[1, 2]; Eliza Lewellyn[1]; Ruth Saecker[1]; Elizabeth Campbell[1]; Seth Darst[1]; Brian T. Chait[1]; [1]*The Rockefeller University, New York, NY;* [2]*Korea Advanced Institute of Science and Technology, Daejeon, South Korea*

MP 477 **Global Analysis of Surfaceome Interaction Network by Integrating Chemical Cross Linking and MS-based Proteomics**; Fangxu Sun[1]; Ronghu Wu[2]; [1]*Georgia Tech, Atlanta, GA;* [2]*Georgia Institute of Technology, Atlanta, GA*

MP 478 **Characterization of high-mass multivalent antigen/antibody complexes by native ESI MS**; Yang Yang[1]; Igor A. Kaltashov[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

MP 479 **Approaching a complete yeast interactome – combining a robust high-throughput pull-down workflow with fast and sensitive Evosep/timsTOF Pro analysis**; André Clemens Michaelis[1]; Andreas-David Brunner[1]; Maximilian Zwiebel[1]; Isabell Bludau[1]; Maximilian T. Strauss[1]; Florian Meier[1]; Matthias Mann[1, 2]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark*

MP 480 **ATF4 Promotes Skeletal Muscle Atrophy by Forming a Heterodimer with CEBPβ**; Scott M. Ebert[1]; Jacob Rose[2]; Steven A. Bullard[1]; Nathan Basisty[2]; George R. Marcotte[1]; Birgit Schilling[2]; Chris Adams[1]; [1]*University of Iowa, College of Medicine, Iowa City, Iowa;* [2]*Buck Institute, Novato, CA*

MP 481 **Our first line of defense: Understanding the mechanism of a novel bactericidal protein using NativeMS**; Anushka Halder[1, 2]; Kallol Gupta[1, 2]; Ryan Gaudet[3, 4, 5]; John Macmicking[3, 4, 5]; [1]*Department of Cell Biology, Yale School of Medicine, New Haven, CT;* [2]*Nanobiology Institute, Yale University, West Haven, CT;* [3]*Howard Hughes Medical Institute, Stanford, CA;* [4]*Departments of Immunobiology and Microbial Pathogenesis, Yale University School of Medicine, New Haven, CT;* [5]*The Systems Biology Institute, Yale University, New Haven, CT*

MP 482 **Investigation into the Mutations Associated with Mohr Syndrome Reveals a critical role for Integrator Proteins**; William K Russell[1]; Lauren G Mascibroda[1]; Eric J Wagner[1]; [1]*University of Texas Medical Branch, Galveston, TX*

MP 483 **RNA Polymerase II Interactome Analysis for Characterization of Transcriptional Elongation Stress**; Dominique A Baldwin[1]; Katlyn D Hughes Burriss[2]; Jose F Victorino[2]; Amber L Mosley[2]; [1]*Indiana University School Of Medicine, Indianapolis, IN;* [2]*Indiana University School of Medicine, Indianapolis, IN*

MP 484 **Platelet factor 4 interactions with heparin oligomers: implications for folding and assembly in vivo**; Chendi Niu[1]; Yang Yang[1]; Igor A. Kaltashov[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

MP 485 **Exposing the heterogeneity of the 20S proteasome by mass spectrometry**; Gili Ben-Nissan[1]; Shay Vimer[1]; Zac Vanaernum[2]; Benjamin J. Jones[2]; Dalton T. Snyder[2]; Vicki H. Wysocki[2]; Yury V. Vasil'ev[3]; Joe S. Beckman[3, 4]; David Morgenstern[1]; Michal Sharon[1]; [1]*Weizmann Institute of Science, Rehovot, Israel;* [2]*Ohio State University, Columbus, Ohio;* [3]*e-MSion Inc., Corvallis, Oregon;* [4]*Oregon State Univeristy, Covallis, Oregon*

MP 486 **A machine learning approach for deciphering protein-protein interactions in human plasma**; Emily Roth[1, 2]; Diane Forget[3]; Vanessa Gaspar[3]; Steffany A. L. Bennett[1, 2]; Marie-Soleil Gauthier[3]; Benoit Coulombe[3, 4]; Mathieu Lavallée-Adam[1, 2]; [1]*University of Ottawa, Ottawa, ON;* [2]*Ottawa Institute of Systems Biology, Ottawa, ON;* [3]*Institut de recherches cliniques de Montréal, Montreal, QC;* [4]*Université de Montréal, Montréal, QC*

MP 487 **The Effect of Ionic Strength on Measured Metalloenzyme-Ligand Binding Constants in Native Mass Spectrometry**; Taylor Perkins[1]; Wonhyeuk Jung[1]; Rachel Ogorzalek Loo[1]; Joseph A. Loo[1]; [1]*UCLA, Los Angeles, CA*

MP 488 **Characterization of DNA Damage, Phosphorylation, and Domain-Specific Interactors of the p53 Transactivation Domains**; Lisa M. Jenkins[1]; Andres Thorkelsson[1]; Sudipto Das[2]; Harichandra D. Tagad[1]; Thorkell Andresson[2]; Ettore Appella[1]; [1]*NIH, Bethesda, MD;* [2]*Frederick National Laboratory for Cancer Research, Frederick, MD*

MP 489 **Hybrid mass spectrometry analysis of multimembrane-spanning efflux pump assemblies**; Tarick J El-Baba[1]; Jani Reddy Bolla[1]; Francesco Fiorentino[1]; Di Wu[1]; Leonhard Urner[1]; Carol V Robinson[1]; [1]*University of Oxford, Oxford, United Kingdom*

MP 490 **Native mass spectrometry and surface-induced dissociation reveal stabilization of Hfq:RNA complexes by intrinsically disordered C-terminal domain**; Samantha H Sarni[1, 2, 3]; Mengxuan Jia[1, 2]; Vicki H Wysocki[1, 2, 3]; Ewelina Malecka-Grajek[4]; Jorjethe Roca[4]; Sarah Woodson[4]; [1]*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, 43210, USA, Columbus, Ohio;* [2]*Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH;* [3]*Ohio State Biochemistry Program, The Ohio State University, Columbus, OH;* [4]*T. C. Jenkins Department of Biophysics, Johns Hopkins University, Baltimore, MD*

MP 491 **Native MS of Protein Complexes: Application of a Next Generation Q-ToF Mass Spectrometer**; Christopher Mallis[1]; Xueyun Zheng[1, 2]; Xi Qiu[3]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX;* [2]*Pacific Northwest National Laboratory, Richland, WA;* [3]*Agilent Technologies, Wilmington, DE*

MP 492   **Quantifying Membrane Protein-Lipid Interactions by Lipid Exchange-Mass Spectrometry**; Guozhi Zhang[1]; Hiruni Jayasekera[1]; James Keener[1]; Michael Thomas Marty[1]; [1]*University of Arizona, Tucson, AZ*

MP 493   **Proximity Ligation by Antibody Recognition for Interactome Studies**; Shujia Dai[1]; Juliane Weißer[2]; Bailin Zhang[1]; [1]*Sanofi, Cambridge, MA; [2]Sanofi, Framingham, MA*

MP 494   **HDX-MS probes respiratory syncytial virus (RSV) antagonism of the host innate immune response**; Nicole D. Wagner[1]; Jingjing Pei[2]; Angela Zou[2]; Gaya K. Amarasinghe[2]; Michael L. Gross[1]; Daisy W. Leung[2]; [1]*Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

MP 495   **Effect of Topo I primary sequence on the conformational dynamics and DNA binding**; Rhyisa C Armbrister; *Florida International University, Miami, FL*

PROTEINS: GENERAL AND MEMBRANE
MP 496-507

MP 496   **Novel Proteomic Approaches to Characterize Endogenous Integral Membrane Protein**; Kyle Brown[1]; Christian Eken[1]; Trisha Tucholski[1]; Song Jin[1]; Ying Ge[1]; [1]*University of Wisconsin, Madison, WI*

MP 497   **Development of lysosome membrane and membrane-binding proteomic strategies both in vitro and in vivo** ; Saadia Hasan[1]; Ashley Frankenfield[2]; Michael Ward[1]; Ling Hao[2]; [1]*National Institute of Neurological Disorders and Stroke, Bethesda, MD; [2]George Washington University, Washington, DC*

MP 499   **High Throughput Native MS With Robust Ion Source Operation for The Analysis of Proteins and Protein Complexes**; Caroline S. Chu[1]; Patrick D. Perkins[1]; Christian Klein[1]; [1]*Agilent Technologies, Santa Clara, CA*

MP 500   **Time-Resolved Analysis of Surface Glycoproteins Unravelling Distinct and Site-Specific Glycosylation Responses of Monocytes and Macrophages to Bacterial Infection**; Suttipong Suttapitugsakul[1]; Ming Tong[1]; Ronghu Wu[1]; [1]*Georgia Institute of Technology, Atlanta, GA*

MP 501   **Establishing proteoliposomes for the analysis of membrane proteins by mass spectrometry**; Melissa Frick[1]; Julian Bender[1]; Carla Schmidt[1]; [1]*Interdisciplinary Research Center HALOmem, Charles Tanford Protein Center, Martin Luther University Halle-Wittenberg, Halle/Saale, Germany*

MP 502   **Mapping Cell Surface Lectin-Glycoprotein Interactions in situ using Oxidation Proteomics**; Yixuan (axe) Xie[1]; Ying Sheng[1]; Qiongyu Li[1]; Seunghye Ju[1]; Joe Reyes[2]; Carlito B Lebrilla[1]; [1]*University of California, Davis, Davis, CA; [2]University of the Philippines, Diliman, Philippines*

MP 503   **CellSurfer Platform for semi-automated cell surface N-glycoprotein profiling of human primary cells reveals cardiomyocyte surface maps**; Linda Berg Luecke[1]; Matthew Waas[2]; Rebekah L. Gundry[2]; [1]*Department of Biochemistry, Medical College of Wisconsin, Milwaukee, WI, 53226; [2]CardiOmics Program, Center for Heart and Vascular Research; Division of Cardiovascular Medicine; and Department of Cellular and Integrative Physiology, University of Nebraska Medical Center, Omaha, NE, 68198*

MP 504   **Investigation of Co-localization of Tagged Surface Proteins by MC-SIMS**; Dmitriy S. Verkhoturov[1]; Michael J. Eller[2]; Yong Duk Han[3]; Stanislav V. Verkhoturov[1]; Alexander Revzin[3]; Emile A. Schweikert[1]; [1]*Texas A&M, College Station, TX; [2]California State University Northridge, Northridge, CA; [3]Mayo Clinic, Rochester, MN*

MP 505   **G protein-coupled receptor (GPCR)-interacting proteins probed by chemical cross-linking and mass spectrometry**; Bill Huang[1]; Hee-yong Kim[1]; [1]*NIAAA/NIH, Rockville, MD*

MP 506   **De Novo Peptide Sequencing from Mass Spectrometry Data with Deep Learning**; Michelle Gill[1]; Joyjit Daw[1]; Johnny Israeli[2]; [1]*NVIDIA, New York, NY; [2]NVIDIA, Santa Clara, CA*

MP 507   **Hydrogen-deuterium Exchange MS elucidates mechanotransmission mechanism of the MacB ABC transporter**; Kjetil Hansen[1]; Nick Greene[2]; Vassilis Koronakis[2]; Argyris Politis[1]; [1]*King's College London, London, United Kingdom; [2]University of Cambridge, Cambridge, United Kingdom*

PROTEINS: PTMS I
MP 509-519

MP 509   **Viral-mediated ubiquitination impacts interactions of host proteins with viral RNA and promotes viral RNA processing**; Christin Herrmann[1, 2]; Jennifer C. Liddle[1, 2]; Joseph M. Dybas[1, 2]; Alexander M. Price[1, 2]; Matthew Charman[1, 2]; Eui Tae Kim[1, 2]; Richard Lauman[2]; Benjamin A. Garcia[2]; Matthew D. Weitzman[1, 2]; [1]*Div. of Protective Immunity and Div. of Cancer Pathobiology, Children's Hospital of Philadelphia, Philadelphia, PA; [2]Dept. of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA*

MP 510   **Discovery of novel citrullination biomarkers in cerebrospinal fluid of patients with Alzheimer's disease**; Zihui Li[1]; Yatao Shi[2]; Bin Wang[2]; Lingjun Li[2]; [1]*University of Wisconsin Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, Wisconsin*

MP 511   **Hydrophilic enhanced dual-functionalized Titanium (IV) IMAC material for enrichment and separation of glycopeptides and phosphopeptides**; Danqing Wang[1]; Junfeng Huang[2]; Min Ma[2]; Lingjun Li[1, 2]; [1]*Department of*

Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705

MP 512　　**Evaluation of enrichment strategies for confident identification of prenylated proteins**; Zixiang Fang[1]; Saiful M. Chowdhury[1]; [1]*University of Texas Arlington, Arlington*

MP 513　　**Ubiquitination promotes protective response to DNA-protein crosslinks**; Luke Erber[1]; Natalia Tretyakova[1]; [1]*University of Minnesota, Minneapolis, MN*

MP 514　　**Characterization of m6A modulation of protein N-terminal methylation and identification of novel N-terminally methylated protein substrates.**; David Bade[1]; Lin Li[2]; Kailin Yu[1]; Xiaoxia Dai[2]; Weili Miao[1]; Yinsheng Wang[1]; [1]*UC Riverside, Riverside, CA; [2]UC RIVERSIDE, Riverside, CA*

MP 515　　**Isomers and Fibrils: Wrenches in the Gears of Lysosomal Digestion**; Tyler R Lambeth[1]; Ryan R. Julian[2]; [1]*University of California-Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

MP 516　　**Phosphoproteome Quantification by TMT and DIA**; Billy W Newton[1]; Yi Zeng[1]; Jia Tang[1]; Guanghui Han[1]; [1]*BGI Americas, San Jose, CA*

MP 517　　**Site-specific Analysis of the Poly-ADP-ribosylated Proteome by Quantitative Mass Spectrometry**; Yonghao Yu; *UT Southwestern Medical Center, Dallas, TX*

MP 518　　**An Integrated Top-Down and Bottom-Up Strategy for Analysis of Bromodomain-containing Protein 4 (BRD4) Mediated Histone Post-Translation Modifications**; Morgan W Mann[1]; Yanlong Zhu[2]; Eli Larson[1]; Ying Ge[1]; Allan R Brasier[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin; [2]University of Wisconsin - Madison, Madison, WI*

MP 519　　**A comprehensive analysis of the human brain acetylome reveals a potential role of acetylation in Alzheimer's disease**; Lidan Sun[1, 2]; Ruchika Bhawal[3]; Hui Xu[1]; Elizabeth Anderson[3]; Sheng Zhang[3]; Gary Gibson[1]; [1]*Weill Cornell Medicine, New York, NY; [2]College of Medicine, Jiaxing University, 314001, China, Jiaxing, China; [3]Cornell University, Ithaca, NY*

PROTEOMICS: INTACT PROTEINS
MP 521-526

MP 521　　**Comparing an intrinsically disordered protein α-synuclein to fixed structure proteins following FPOP modification using high resolution LCMS intact analysis**; Alan Barnes[1]; Jake A Busuttil-Goodfellow[2]; James Ault[2]; Neil J Loftus[1]; Frank Sobott[2]; [1]*Shimadzu MS/BU, Manchester, United Kingdom; [2]University of Leeds, Leeds, United Kingdom*

MP 522　　**Unravelling hundreds of proteoforms of heavily glycosylated enzymes using native-like LC-MS analysis**; Michiel Akeroyd[1]; Olaf Schouten[1]; Stephane Bahraoui[2]; Marshall Bern[2]; [1]*DSM Biotechnology Center, Delft, Netherlands; [2]Protein Metrics Inc, Cupertino, CA*

MP 523　　**Capillary chromatography for intact therapertic proteins and their subunit analyses using MAbPac RP column**; Xuefei Sun[1]; Zoltan Szabo[1]; Brandon H. Robson[1]; Shanhua Lin[1]; Mike Baynham[2]; Rainer Bauder[3]; [1]*Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, Runcorn, United Kingdom; [3]Thermo Fisher Scientific, Cambridge, MA*

MP 524　　**Intact analysis and binding site determination of covalent ibrutinib adduct with human serum proteins by LC-triple TOF mass spectrometer**; Ming Yao[1]; Jinping Gan[2]; [1]*Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb Company, Princeton, NJ*

MP 525　　**Automating the characterization of ambiguity in proteoform identifications with discovery top-down proteomics**; Richard Leduc[1]; Ryan Fellers[2]; Bryan P Early[2]; Joe Greer[2]; Paul Thomas[2]; Michael R. Shortreed[3]; Lloyd M. Smith[3]; Neil L Kelleher[2]; [1]*Northwestern University, Bloomington, IN; [2]Northwestern University, Evanston, IL/60208; [3]University of Wisconsin-Madison, Madison, Wisconsin*

MP 526　　**Aging in the mouse brain is associated with increased histone methylation on histone H3.3**; Karl Poncha[1]; Tao Wang[2]; Matthew Holt[2]; Nicolas L. Young[2]; [1]*BCM, Houston; [2]BCM, Houston, Texas*

PROTEOMICS: NEW APPROACHES I
MP 527-541

MP 527　　**Development of an Efficient Method for Biotinylated Protein Purification Coupled with Tandem Mass Tag Mass Spectrometry**; Huan Sun[1]; Xiaojun Sun[1]; Junmin Peng[1, 2]; [1]*Departments of Structural Biology and Developmental Neurobiology, St. Jude Children's Research Hospital, Memphis, TN; [2]Center for Proteomics and Metabolomics, St. Jude Children's Research Hospital, Memphis, TN*

MP 528　　**GlobeQuant-A method for Proteome-wide absolute quantification**; Bharath Kumar Raghuraman[1]; Ignacy Rzagalinski[1]; Andrej Shevchenko[1]; [1]*Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany*

MP 529 **Chemical probe with α-methylene-β-lactone warhead labeling diverse classes of enzymes**; Lei Wang[1]; Louis P. Riel[1]; Bekim Bajrami[2]; Bin Deng[3]; Amy R. Howell[1]; Xudong Yao[1]; [1]*Department of Chemistry, University of Connecticut, Storrs, CT;* [2]*Chemical Biology & Proteomics, Biogen, Cambridge, MA;* [3]*Department of BIology, University of Vermont, Burlington, VT*

MP 530 **Robust, reproducible and quantitative analysis of thousands of proteomes by micro-flow LC-MS/MS**; Yangyang Bian[1]; Runsheng Zheng[1]; Florian P Bayer[1]; Cassandra Wong[2]; Yun-Chien Chang[1]; Chen Meng[3]; Daniel P Zolg[1]; Maria Reinecke[1]; Jana Zecha[1]; Svenja Wiechmann[1]; Stephanie Heinzlmeir[1]; Johannes Scherr[4]; Bernhard Hemmer[5]; Mike Baynham[6]; Anne-Claude Gingras[2]; Oleksandr Boychenko[7]; Bernhard Kuster[1]; [1]*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany;* [2]*Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ontario;* [3]*Bavarian Biomolecular Mass Spectrometry Center (BayBioMS), Technical University of Munich, Freising, Germany;* [4]*Centre for Preventive and Sports Medicine, Klinikum Rechts der Isar, Technical University of Munich, Munich, Germany;* [5]*Department of Neurology, Klinikum Rechts der Isar, Medical Faculty, Technical University of Munich,, Munich, Germany;* [6]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [7]*Thermo Fisher Scientific, Germering, Germany*

MP 531 **Bead Assisted Mass Spectrometry (BAMS™) Enables Effectively Instantaneous Transformation of MS1 Peak Lists to Quantitative Pathway Reports**; Sergey Mamaev[1]; Manor Askenazi[2]; Camilla Worsfold[1]; Jeffery C. Silva[1]; Vladislav B. Bergo[1]; [1]*Adeptrix Corporation, Beverly, MA 01915;* [2]*Biomedical Hosting LLC, Arlington, MA 02474*

MP 532 **Expanding Proteome Coverage through the Use of Lysobacter Capsici beta-lytic Metalloendopeptidase**; Mikhail Konstantinov[1]; Alexey Afoshin[2]; Irina Kudryakova[2]; Natalia Vasilyeva[2]; Ilya Toropygin[3]; [1]*Orekhovich Institute of Biomedical Chemistry, Moscow, Russia;* [2]*G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Pushchino, Russia;* [3]*Inst.of Biomedical Chemistry, Moscow, Russian Federation*

MP 533 **The Julienne method improves depths of proteome coverage and LCMS throughput**; Thomas Clark[1]; Queenie Chen[1]; Nik Stoynov; Greg Stacey[1]; Karina Nielsen[1]; Michael Skinnider[1]; Leonard Foster[1]; [1]*UBC, Vancouver, BC*

MP 534 **Absolute Quantitation of Proteins by Coulometric Mass Spectrometry**; Pengyi Zhao[1]; Qi Wang[1]; Manpreet Kaur[1]; Yong-Ick Kim[1]; Howard D Dewald[2]; Hao Chen[1]; [1]*New Jersey Institute of Technology, Newark, NJ;* [2]*Ohio University, Athens, OH*

MP 535 **Heat and Beat (HnB): A one-pot rapid tissue sample preparation technique for proteomics in under an hour**; Dylan Xavier[1]; Clare Loudon[1]; Peter G Hains[1]; Philip J Robinson[1, 2]; [1]*Children's Medical Research Institute, Westmead, Australia;* [2]*University of Sydney, Camperdown, Australia*

MP 536 **Trypsin Limited Proteolysis Strategy towards in-depth Structural Proteomics**; Kosuke Ogata[1]; Yasushi Ishihama[1]; [1]*Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*

MP 537 **ClpCP in the act: Degradomics investigation of ClpCP-substrates**; David Mario Hoi[1, 2]; Julia Leodolter[1]; Markus Hartl[2]; Tim Clausen[1]; [1]*Institute of Molecular Pathology (IMP), Vienna, Austria;* [2]*Max Perutz Labs, Vienna, Austria*

MP 538 **Turnkey, multi-pathway signaling analysis using a synthetic phosphopeptide panel, standardized sample preparation kits and SureQuant internal standard targeted quantitation**; Aaron S Gajadhar[1]; Bhavin Patel[2]; Penny Jensen[2]; Sebastian Gallien[3, 4]; Romain Huguet[5]; Kay Opperman[2]; John C Rogers[2]; Andreas Huhmer[5]; Daniel Lopez-Ferrer[5]; [1]*Thermo Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Rockford, IL;* [3]*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA;* [4]*Thermo Fisher Scientific, Paris, France;* [5]*Thermo Fisher Scientific, San Jose, CA*

MP 539 **Comprehensive and robust proteome profiling using Online-2D nanoLC coupled to the Orbitrap Exploris 480 MS**; Tabiwang N. Arrey[1]; Runsheng Zheng[2]; Oleksandr Boychenko[2]; Alexander Harder[3]; [1]*Thermo Fisher Scientific, Bremen, Germany;* [2]*Thermo Fisher Scientific, Germering, Germany;* [3]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 540 **Robust Label-Free Proteomics Analysis with a New Orbitrap Mass Spectrometer, FAIMS Separation and micro- Pillar Array columns (uPAC) chromatography**; Khatereh Motamedchaboki[1]; Aaron S. Gajadhar[2]; Aman Makaju[2]; Yang Liu[2]; Julia Kraegenbring[3]; Tabiwang N. Arrey[3]; Geert Van Raemdonck[4]; Ali Pervez[4]; David M Horn[2]; Alexander Harder[3]; Daniel Lopez-Ferrer[2]; [1]*thermo fisher scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, San Jose, California;* [3]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* [4]*PharmaFluidics, Technologiepark-Zwijnarde 82, Gent, Belgium*

MP 541 **Deep proteome coverage and label-free proteomic analysis of low numbers of mammalian cells with a quadrupole-ion-trap-Orbitrap mass spectrometer**; Min Huang[1]; Xiujie Sun[1]; Yue Zhou[1]; [1]*Thermo Fisher Scientific, Shanghai, China*

SINGLE CELL MS
MP 542-568

MP 542   **A Microfluidic Platform Enabling In Situ Bioreactor Monitoring and Single Cell-Scale Biomarker Discovery Using ESI-MS**; Austin L. Culberson[1]; Mason A. Chilmonczyk[1]; Peter A. Kottke[1]; Andrei G. Fedorov[1, 2]; [1]*The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA;* [2]*Parker H. Petit Institute for Bioengineering & Biosciences, Georgia Institute of Technology, Atlanta, GA*

MP 543   **Single cell HbA1C measurement using isotope dilution mass spectrometry to determine erythrocyte age**; Azad Eshghi[1]; Darryl Hardie[1]; Ying Zhu[2]; Ryan T Kelly[2, 3]; David R Goodlett[4, 5]; [1]*uvic genome bc protein centre, victoria;* [2]*Pacific Northwest National Lab, Richland, WA;* [3]*Brigham Young University, Provo, UT;* [4]*University of Maryland, Balitmore, Baltimore, MD;* [5]*University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland*

MP 544   **Single Cell Proteomics and the Carrier Proteome Effect**; Bernhard Kuster[1]; Christopher M. Rose[2]; [1]*Proteomics and Bioanalytics, Technical University of Munich, Germany;* [2]*Discovery Proteomics, Genentech Inc., So. San Francisco, CA*

MP 545   **Cell Classification Using Single Cell Mass Spectrometry Through Interpretable Machine Learning**; Yuxuan Xie[1]; Daniel C Castro[1]; Sara E Bell[1]; Stanislav Rubakhin[1]; Jonathan V Sweedler[1]; [1]*University of Illinois at Urbana-Champaign, Urbana, IL*

MP 546   **Integration of patch-clamp electrophysiology with single-cell mass spectrometry for proteomic analysis to extend the bioanalytical toolbox of neuroscience**; Sam Choi[1]; Peter Nemes[1]; Abigail Polter[2]; [1]*University of Maryland College Park, College Park, MD;* [2]*George Washington University, Washington, DC*

MP 547   **PASEF for sensitive shotgun proteomics: toward single cell analysis**; Thomas Kosinski[1]; Ning Chen[2]; Markus Lubeck[1]; Heiner Koch[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Bruker (Beijing) Scientific Technology Co., Ltd., Beijing, China*

MP 548   **High Sensitivity Top-Down Proteomics of Single Muscle Fibers**; Jake A. Melby[1]; Yutong Jin[2]; Kyle Brown[2]; Yanlong Zhu[2]; Ziqing Lin[2]; Gary Diffee[2]; Ying Ge[2]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*University of Wisconsin-Madison, Madison, Wisconsin*

MP 549   **A highly sensitive and precise analytical method for mitochondrial metabolites using LC-MS/MS with a photo-affinity reaction**; Hajime Mizuno[1]; Natsumi Tanaka[1]; Takamitsu Sasaki[1]; Iwao Sakane[2]; Eiji Sugiyama[1]; Toshimasa Toyo'oka[1]; Kouichi Yoshinari[1]; Shinobu Kudoh[3]; Kenichiro Todoroki[1]; [1]*University of Shizuoka, Shizuoka, Japan;* [2]*ITO-EN LTD, Tokyo, Japan;* [3]*Yokogawa Electric Corporation, Musashino, Japan*

MP 550   **Improved single-cell neuronal proteome coverage by integration of nanoPOTS and SMTA chemical labeling mass spectrometry**; Santosh A. Misal[1]; Amanda J. Guise[2]; Yongzheng Cong[1]; Edward D. Plowey[2]; Samuel Payne[1]; Ryan T. Kelly[1]; [1]*Brigham Young University, Provo, UT;* [2]*Biogen, Inc., Cambridge, Massachusetts*

MP 551   **Toward Low-Input Metabolomics using Microfluidic Sample Preparation**; Steven R Doonan[1]; Gary Patti[1]; [1]*Washington University in St. Louis, St. Louis, MO*

MP 552   **Automating nanodroplet sample preparation with liquid chromatography-mass spectrometry for high throughput single-cell proteomics**; Sarah M Williams[1]; Andrey Liyu[1]; Chia-Feng Tsai[1]; Ronald J. Moore[1]; Daniel J. Orton[1]; William B. Chrisler[1]; Gaffrey J. Mathew[1]; Tao Liu[1]; Ryan T. Kelly[2]; Richard D. Smith[1]; Ljiljana Pasa-Tolic[1]; Ying Zhu[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Brigham Young University, Provo, UT*

MP 553   **Single-cell proteomic analysis combining nanoPOTS, nanoLC and FAIMSpro increases coverage to >1000 proteins/cell**; Yongzheng Cong[1]; Khatereh Motamedchaboki[2]; Santosh A. Misal[1]; Yiran Liang[1]; Amanda J. Guise[3]; Thy Truong[1]; Yufeng Shen[4]; Romain Huguet[2]; Daniel Lopez-Ferrer[2]; Edward D. Plowey[3]; Ying Zhu[5]; Ryan T. Kelly[1, 5]; [1]*Brigham Young University, Provo, UT;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Biogen, Inc., Cambridge, Massachusetts;* [4]*CoAnn Technologies, LLC, Richland, Washington;* [5]*Pacific Northwest National Laboratory, Richland, WA*

MP 554   **Comprehensive Single Cell and Bulk Proteomic Analyses of Human Cellular Models for HIV Reactivation**; Soham Gupta[1]; Jimmy E Rodriguez[1]; Ujjwal Neogi[1]; Roman A Zubarev[1]; Akos Vegvari[1]; [1]*Karolinska Institutet, Stockholm, Sweden*

MP 555   **Single-Cell Deep Lipidomics via Photochemical Reaction and Tandem Mass Spectrometry**; Zishuai Li[1]; Simin Cheng[1]; Qiaohong Lin[1]; Wenbo Cao[1]; Jing Yang[1]; Wenpeng Zhang[1]; Yu Xia[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; [1]*Tsinghua University, Beijing, China*

MP 556   **Single-Cell Proteome Signatures – Comparative Protein Expression Profiles from Ultra-low Input Samples by combining TMT and Data-Independent Acquisition Strategies**; Claudia Ctortecka[1, 2]; Gabriela Krššáková[1]; Florian Stanek[1]; Karel Stejskal[2]; Josef M. Penninger[2, 3]; Karl Mechtler[1, 2]; Johannes Stadlmann[2]; [1]*IMP, Vienna, Austria;* [2]*Institute of Molecular Biotechnology, Austrian Academy of Sciences (IMBA), Vienna, Austria;* [3]*Department of Medical Genetics, Life Sciences Institute, University of British Columbia, Vancouver, BC*

MP 557   **Quantification of the Emergence of Macrophage Heterogeneity by Single-Cell Proteomics**; Harrison Specht[1]; Edward Emmott[1]; Aleksandra Petelski[1]; R. Gray Huffman[1]; Hendrik Wesseling[2]; Marco Serra[3]; Peter Kharchenko[3]; Erik Hett[2]; David H Perlman[2]; Antonius Koller[1]; Nikolai Slavov[1]; [1]*Department of Bioengineering and Barnett*

Institute, Northeastern University, Boston, MA; [2]Merck Exploratory Sciences Center, Merck Sharp & Dohme Corp, Cambridge, MA; [3]Department of Biomedical Informatics, Harvard Medical School, Boston, MA

MP 558   **Determination of double-bond position in unsaturated lipids: reactive single cell mass spectrometry studies**; Yanlin Zhu[1]; Wenhua Wang[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

MP 559   **Single Cell MS Metabolomics Studies of Anticancer drug-resistant Cells: understanding synergetic effect of mono- and combinational treatments**; Xingxiu Chen[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

MP 560   **Pushing the Limits of Sensitivity: Micropillar Array-Based Chromatography Coupled to a Quadrupole Orbitrap Mass Spectrometer and FAIMS for Low-Input Proteomics**; Julia Kraegenbring[1]; Karel Stejskal[2]; Otto Hudecz[2]; Gabriela Krssakova[2]; Jeff Op De Beeck[3]; Tabiwang N. Arrey[4]; Bernard Delanghe[4]; Alexander Harder[4]; Karl Mechtler[2, 5]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Institute of Molecular Biotechnology, Austrian Academy of Sciences (IMBA), Vienna, Austria; [3]PharmaFluidics, Technologiepark-Zwijnarde 82, Gent, Belgium; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [5]IMP, Vienna, Austria*

MP 561   **Exploratory approaches to highly-sensitive analysis toward single-cell shotgun proteomics using nano-LC/MS/MS**; Kosuke Hata[1]; Takeshi Hara[1]; Yoshihiro Izumi[1]; Masaki Matsumot[1, 2]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Department of Omics and Systems Biology, Graduate School of Medical and Dental Sciences Niigata University, Niigata, Japan*

MP 562   **High throughput, single cell proteomics analysis by multiplexed, miniaturized Filter Aided Sample Preparation method (MICRO-FASP)**; Zhenbin Zhang[1]; Norman Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN*

MP 563   **Comparative MALDI MS analysis of human pancreatic islets – from tissues to individual cells**; Stanislav Rubakhin[1]; Jonathan V Sweedler[2]; *[1]Beckman Institute, UIUC, Urbana, IL; [2]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL*

MP 564   **High Precision UV Ablation Sampling for MALDI Mass Spectrometry**; Kelcey B Hines[1]; Fabrizio Donnarumma[2]; Kermit K. Murray[2]; *[1]Louisiana State University, Baton Rouge, LA; [2]Louisiana State University, Baton Rouge, LOUISIANA*

MP 565   **Evaluation of solid-phase extraction-based sample processing techniques for ultra-sensitive deep proteomic profiling of limited samples using ultra-low flow LC-MS/MS**; Jan Schejbal[1]; Michal Gregus[1]; James Kostas[1]; Joanna Lee[1]; Alexander R. Ivanov[1]; *[1]Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA*

MP 566   **Sensitive and high-throughput single-cell proteomics workflow on new quadrupole-ion trap-Orbitrap mass spectrometer with FAIMS separation**; Khatereh Motamedchaboki[1]; Maowei Dou[2]; Yongzheng Cong[3]; Romain Huguet[4]; Aaron M Robitaille[5]; Yufeng Shen[6, 7]; Daniel Lopez-Ferrer[8]; Ryan T. Kelly[3]; Ying Zhu[9]; *[1]thermo fisher scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL; [3]Brigham Young University, Provo, UT; [4]Thermo Fisher Scientific, San Jose, California; [5]Thermo Fisher Scientific, San Jose, CA; [6]CoAnn Technologies LLC, Richland, WA; [7]CoAnn Technologies, LLC, Richland, Washington; [8]ThermoFisher Scientific, San Jose, CA; [9]Pacific Northwest National Laboratory, Richland, WA*

MP 567   **Single Cell-ICP-MS, an Emerging Technology to Study Microorganisms**; Honglan Shi; *Missouri University of Sciense and Technology, Rolla, MO*

MP 568   **Single-cell metabolomics of hydrophilic metabolites in typical mammalian cells based on highly sensitive nano-liquid chromatography tandem mass spectrometry**; Kohta Nakatani[1]; Yoshihiro Izumi[1]; Kosuke Hata[1]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan*

TOXICOLOGY
MP 569-581

MP 569   **Multiplex Quantitation of Biomolecules Involved in Copper Toxicity via Custom N,N-Dimethylated Leucine (DiLeu) 12-plex Isobaric Tags**; Christopher S Sauer[1]; Mason A Job[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 570   **Development and Application of an LC/MS/MS Method for Evaluation of Xenobiotic Disruption of In Vitro Thyroid Hormone Metabolism**; Denise Macmillan[1]; Mihaela Mocanu[2]; Joseph Strasser[2]; Vicki M. Richardson[1]; *[1]USEPA/ORD/CCTE, Durham, NC; [2]Oak Ridge Institute for Science and Education (ORISE) Participant Program, Durham, NC*

MP 571   **Identification of Aflatoxin transformation products in standards and corn after high voltage atmospheric cold plasma treatment using an Orbitrap ID-X**; Dwayne E Schrunk[1]; Laura E Burns[1]; Scott Peterman[2]; Caroline Ding[2]; Brandon Bills[2]; Ed George[2]; Kizito Nishimwe[1]; Graeme Mcalister[2]; Seema Sharma[2]; *[1]Iowa State University, Ames, IA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 572   **Multi-target screening of toxicological compounds in blood on a fully-automated platform consisting of sample preparation module CLAM and LC-MS/MS**; Nat Tansrisawad[1]; Udomsak Hoonwijit[1]; Apinya

Tubtimrattana[2]; Boontariga Intawong[1]; Samita Tanasarnsopaporn[2]; Jakkapan Boonsritan[1]; Zhe Sun[3]; Chukkapong Comsup[4]; Prapath Tienprateep[4]; <u>Zhaoqi Zhan</u>[3]; [1]*Department of Forensic Medicine, Chulalongkorn University, Bangkok, Thailand;* [2]*Department of Forensic Medicine, King Chulalongkorn Memorial Hospital, The Thai Red Cross Society, Bangkok, Thailand;* [3]*Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore;* [4]*Bara Scientific Co., Ltd,, Bangkok, Thailand*

MP 573   **Urine LDTD-MS/MS Drugs of Abuse Screening in Urine at 9 Seconds per Sample Using Dry-and-Dissolve preparation**; <u>Jonathan Rochon</u>[1]; Jean Lacoursière[2]; Serge Auger[2]; Francis Brière[1]; Pier-Luc Plante[1]; Pierre Picard[2]; [1]*Université Laval, Québec, QC;* [2]*Phytronix Technologies, Inc., Quebec, QC*

MP 574   **An SLE-Based Workflow for the Analysis of the SAMHSA Oral Fluid Drug List by LC/TQ**; <u>Jennifer Cottine Hitchcock</u>[1]; Tina Chambers[1]; Andre Szczesniewski[1]; [1]*Agilent Technologies, Santa Clara, CA*

MP 575   **Simultaneous determination of nicotine, cocaine, opioids, caffeine, and metabolites in human brain and placenta by LC-MS/MS**; <u>Tian Liu</u>[1]; Dominique B Figueroa[2]; Maureen A Kane[1]; [1]*University of Maryland, Baltimore, Baltimore, MD;* [2]*University of Maryland, Balitmore, Baltimore, MD*

MP 576   **Monitoring the Human Hemoglobin and Human Serum Albumin Adductome in Contact Allergy**; <u>Lorena Ndreu</u>[1]; Luke Erber[2]; Andrew Rajczewski[2]; Margareta Törnqvist[1]; Natalia Tretyakova[2]; Leopold Ilag[1]; Isabella Karlsson[1]; [1]*Stockholm University, Stockholm, Sweden;* [2]*University of Minnesota Masonic Cancer Center, Minneapolis, MN*

MP 577   **Expanding capabilities in routine clinical toxicology screening using HRAM QTOF**; <u>Simon Ashton</u>[1]; Tiphaine Robin[2]; Alan Barnes[1]; Emily Armitage[1]; Neil J Loftus[1]; Sylvain Dulaurent[3]; Pierre Marquet[3]; Souleiman El Balkhi[3]; Franck Saint-Marcoux[3]; [1]*Shimadzu MS/BU, Manchester, United Kingdom;* [2]*Shimadzu France, Paris, France;* [3]*CHU Limoges, Limoges, France*

MP 578   **Controlling Crosstalk of Amphetamine and Methamphetamine in Urine Assays Using 96 well plates for LC-MS/MS Analysis**; <u>Stephanie Marin</u>[1]; Mario Merida Iii[1]; Jeremy Smith[1]; Elena Gairloch[1]; [1]*Biotage, Charlotte, NC*

MP 579   **Rapid Detection of Growth Hormone-Releasing Peptides in Dried Blood Spots**; Pierre Negri[1]; <u>Enrico Gerace</u>[2]; Jessica Modaffari[2]; Daniele Dicorcia[2]; Marco Vicenti[2, 3]; Alberto Salomone[2, 3]; [1]*SCIEX, Redwood City, CA;* [2]*Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Turin, Italy;* [3]*Dipartimento di Chimica, Universita' degli Studi di Torino, Torino, Italy*

MP 580   **Detection of Fentanyl Analogs and Novel Synthetic Opioids in Hair**; Pierre Negri[1]; <u>Daniele Dicorcia</u>[2]; Alberto Salomone[2]; [1]*SCIEX, Redwood City, CA;* [2]*Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Turin, Italy*

MP 581   **Rapid Detection of Isomeric Fentanyl Analogs at Trace Levels using LC-TIMS-TOF MS**; <u>Elisa N Shoff</u>[1, 2]; Cesar E. Ramirez[2]; Francisco A. Fernandez-Lima[2]; [1]*Miami-Dade Medical Examiner Department, Miami, FL;* [2]*Florida International University, Miami, FL*

AMBIENT IONIZATION: APPLICATIONS II
TP 001-020

TP 001   **Identification of Tryptophan Metabolites in Brain Tissue Using Paper Spray Ionization-Mass Spectrometry**; Marco V Melgar[1]; Richard C Dilworth[1]; Vanessa Y Rubio[1]; Gary P Wang[1]; Timothy J Garrett[1]; *University of Florida, Gainesville, FL*

TP 002   **Ultrasonic Nebulizer Assisted Atmospheric-Pressure Chemical Ionization (APCI) for Explosives analysis**; Linxia Song[1]; Theresa Evans-Nguyen[1]; *University of South Florida, Tampa, FL*

TP 004   **Ultrafast qualitative screening of mitragynine, MDMA, and tetrahydrocannabinol (THC) in complex matrices by green technology direct probe ionization mass spectrometry**; Udi Jumhawan[1]; Saravana Kumar Jayaram[2]; May Yen Ang[3]; Hazni Hashim[3]; Muhammad Hafis Zulkiflee[2]; Nur Nazihah Md Shahari[2]; Wan Rahimah Wan Ahmad[2]; Sandhya Aniruddha Nargund[1]; Lai Chin Hui-Loo[1]; *Shimadzu Asia Pacific, Singapore, Singapore; 2Division of Narcotics, Department of Chemistry Malaysia, Petaling Jaya, Malaysia; 3Shimadzu Malaysia, Petaling Jaya, Malaysia*

TP 005   **Thermal Desorption Enabled Electrospray and DART Ionization of Solids and Inorganic Salts**; Frederick Li[1]; Paul Liang[1]; Scott Oro[1]; Brittany Laramee[1]; Kenyon Evans-Nguyen[2]; Brian Musselman[1]; *IonSense,Inc., Saugus, MA; 2University of Tampa, Tampa, FL*

TP 006   **Skip Sample Preparation and Facilitate Analysis of Food by Screening via the 24-Pin Sampler with DART-MS**; Brittany Laramee[1]; Frederick Li[1]; Paul Liang[1]; Brian Musselman[1]; *IonSense, Inc, Saugus, MA*

TP 007   **Real-Time Monitoring of Cellular Metabolism by Dual-Probe Microsampling Integrated with Multiplexed Ion Mobility-Mass Spectrometry**; Taylor M Domenick[1]; Richard A Yost[1]; Vinata Vedam-Mai[1]; *University of Florida, Gainesville, FL*

TP 008   **Microdroplet-accelerated Synthesis of Substituted Benzimidazoles**; Pallab Basuri[1, 2]; L. Edwin Gonzalez[1]; Thalappil Pradeep[2]; R. Graham Cooks[1]; *Purdue University, West Lafayette, IN; 2Indian Institute of Technology, Madras, Chennai, India*

TP 009   **Mass spectrometry analysis reveals metabolic discrepancies between histologically equivalent tissues that may hamper utility in molecular profiling**; Michael Woolman[1]; Lauren Katz[1]; Georgia Gopinath[1]; Taira Kiyota[2]; Claudia Kuzan-Fischer[1]; Isabelle Ferry[1]; Megan Wu[1]; Sunit Das[1]; Michael D Taylor[1]; James Rutka[1]; Howard Ginsberg[1]; Ahmed Aman[2]; Arash Zarrine-Afsar[1]; *University of Toronto, Toronto, ON; 2Ontario Institute for Cancer Research, Toronto, ON*

TP 010   **Post-acquisition Data Analysis Program for Automating Data Processing in High-throughput Experimentation with DART-MS**; Robert Goguen[1]; Frederick Li[1]; Paul Liang[1]; Brittany Laramee[1]; Brian Musselman[1]; *IonSense, Inc, Saugus, MA*

TP 011   **Diagnosis of metabolic diseases by discriminative biofluid fingerprinting: reaching the next level with laser-assisted rapid evaporative ionization mass spectrometry (LA-REIMS)**; Lieven Van Meulebroek[1]; Ellen De Paepe[1]; Kathleen Wijnant[1, 2]; Vera Plekhova[1]; Margot De Spiegeleer[1]; Bruno Lapauw[3]; Nathalie Michels[2]; Stefaan De Henauw[2]; Myriam Van Winckel[4]; Lynn Vanhaecke[1, 5]; *Ghent University, Faculty of Veterinary Sciences, Merelbeke, Belgium; 2Ghent University, Faculty of Medicine and Health Sciences, Ghent, Belgium; 3Ghent University Hospital, Department Endocrinology, Ghent, Belgium; 4University Hospital Ghent, Department Pediatrics and Medical Genetics, Ghent, Belgium; 5Queen's University, Institute for Global Food Security, Belfast, United Kingdom*

TP 012   **In situtissue pathology from spatially encoded mass spectrometry classifiers visualized in real time through augmented reality**; Michael Woolman[1]; Jimmy Qiu[2]; Claudia Kuzan-Fischer[1]; Isabelle Ferry[1]; Delaram Dara[1]; Lauren Katz[1]; Fowad Daud[1]; Megan Wu[1]; Manuela Ventura[2]; Nicholas Bernards[2]; Harley Chan[2]; Inga Fricke[2]; Mark Zaidi[1]; Michael D Taylor[1]; James Rutka[1]; Sunit Das[1]; Jonathan Irish[2]; Robert Weersink[2]; Howard Ginsberg[1]; David Jaffray[2]; Arash Zarrine-Afsar[1]; *University of Toronto, Toronto, ON; 2University Health Network, TORONTO, ON*

TP 013   **High-throughput assay and intact protein analysis by liquid AP-MALDI MS**; Henriette Krenkel[1]; Evita Hartmane[1]; Cristian Piras[1]; Jeffery Brown[1, 2]; Michael Morris[2]; Rainer Cramer[1]; *University of Reading, Reading, United Kingdom; 2Waters Corporation, Wilmslow, United Kingdom*

TP 014   **Application of VeriSpray ion source Triple Quadrupole Mass Spectrometry for the analysis of stimulants and narcotics in oral fluid**; Gustavo de Albuquerque Cavalcanti[1]; Yu Zhu[2]; Wijeratne Neloni[2]; Claudia Martins[3]; *Brazilian Doping Control, Rio de Janeiro, Brazil; 2Thermo Fisher Scientific, San Jose, CA; 3ThermoFisher Scientific, San Jose, CA*

TP 015   **Rapid Screening of High Priority N-Nitrosamines in Pharmaceutical, Forensic, and Environmental Samples with FCSI-MS and PSI-MS**; Trevor J. McDaniel[1]; Jessica M. Holtz[1]; Makoy Overfelt[1]; Christopher C. Mulligan[1]; *Illinois State University, Normal, IL*

TP 016   **Rapid Analysis of Products from High Throughput Exerimentation Utilizing a Novel Pulsed Gas Control System for an Ambient Ionization Source**; <u>Brian D. Musselman</u>[1]; Paul Liang[2]; Scott Oro[2]; Brittany Laramee[2]; Frederick Li[2]; [1]*IonSense, Inc., Saugus, MA*; [2]*IonSense, Inc, Saugus, MA*

TP 017   **Rapid screening procedures for a wide variety of forensic samples using an ambient ionization technique coupled to different mass spectrometers**; <u>Eshwar Jagerdeo</u>[1]; Serge Auger[2]; [1]*FBI, Springfield, VA*; [2]*Phytronix Technologies, Inc., Quebec, QC*

TP 018   **Rapid Detection of 25 Types of Drugs by DART Coupled with Ultivo Triple Quadrupole MS**; <u>Jianzhong Li*</u>[1]; Kerry Song[2]; Xiaokun Duan[2]; [1]*Agilent Technologies, Beijing, China*; [2]*ASPEC Technologies, Beijing, China*

TP 019   **Identification of Random or Block Copolymers by Pyrolysis DART-MS: A Comparison Study with Pyrolysis GC-MS**; <u>Ruilin Hu*</u>[1]; Dongyan Mao[1]; Xiaokun Duan[2]; Kerry Song[2]; Charles C. Liu[2]; [1]*BASF Advanced Chemicals Co., Ltd., Shanghai, China*; [2]*ASPEC Technologies, Beijing, China*

TP 020   **Pulse DART: Improving Throughput and Reducing Helium Consumption, Ambient Background and Matrix Interference**; <u>Scott Oro</u>[1]; Frederick Li[2]; Paul Liang[2]; Brittany Laramee[2]; Brian Musselman[2]; [1]*IonSense, Saugus, MA*; [2]*IonSense, Inc, Saugus, MA*

ANTIBODIES & ANTIBODY DRUG CONJUGATES II
TP 022-035

TP 022   **The HOS and thermal stability of six biotherapeutic antibodies based on mobility measurements of singly-charged electrospray ions at atmospheric pressure**; <u>Henry Benner</u>[1]; Ben Aguilar[1]; [1]*Ion Dx, Monterey, CA*

TP 023   **Profiling in vivo and in vitro Biotransformation of Biotherapeutics by Immunoaffinity LC-MS/MS**; <u>Suk-Joon Hyung</u>[1]; Surinder Kaur[1]; Ola Saad[1]; [1]*Genentech, South San Francisco, CA*

TP 024   **Development of a New Workflow for Multiple Attribute Monitoring (MAM) of an Antibody-Drug-Conjugate (ADC)**; <u>Armelle Martelet</u>[1]; Valérie Garrigue[1]; Hélène Le Borgne[1]; Bruno Genet[1]; Zoe Zhang[2]; Kerstin Pohl[3]; [1]*SANOFI, Vitry sur seine, France*; [2]*SCIEX, Redwood Shores, CA*; [3]*Sciex, Framingham, MA*

TP 025   **Implementing MHC Associated Peptide Proteomics (MAPPs) in drug development and immunogenicity risk assessment**; <u>Jason Lamar</u>[1]; Sylvia Wong[2]; Violet Lee[2]; Lynn Kamen[2]; Ben Ordonia[2]; Azadeh Hassanzadeh[2]; Shan Chung[2]; Surinder Kaur[2]; Ola Saad[2]; [1]*Genentech - South San Francisco, CA, SSF, CA*; [2]*Genentech, South San Francisco, CA*

TP 026   **Automated affinity capture LC-MS methods for bioanalysis of Antibody Drug Conjugates (ADCs) and antibody fusion proteins**; <u>Madhura Deshpande</u>[1]; Srikanth Kotapati[1]; Aarti Jashnani[1]; Jason Hogan[1]; Gavin Dollinger[1]; Arvind Rajpal[1]; [1]*Bristol-Myers Squibb, Redwood City, CA*

TP 027   **High resolution LC/MS characterization of site-specific antibody-drug conjugate synthesized by CCAP method**; <u>Kenji Hirose</u>[1]; Taiji Kawase[1]; Satoshi Kishimoto[2]; Takaaki Hatanaka[2]; Motoyasu Adachi[3]; Yuji Ito[2]; [1]*Nihon Waters K.K., Osaka, Japan*; [2]*Kagoshima University, Kagoshima, Japan*; [3]*National Institutes for Quantum and Radiological Science and Technology, Ibaraki, Japan*

TP 028   **A novel method for Identification of Monoclonal antibodies from Hybridoma Supernatants using Reverse Immunocapture LC-MS/MS**; <u>Kristin Geddes</u>[1]; Yaping Liu[2]; Eberhard Durr[2]; Arthur Fridman[2]; Zhifeng Chen[2]; Toya Nath Baral[3]; Daniel S Spellman[2]; [1]*Merck & Co., Inc., West Point, PA*; [2]*Merck and Co, Inc, West Point, PA*; [3]*Merck & Co., Inc., South San Francisco, CA*

TP 029   **Reproducibility of native SEC LC-MS intact mAb characterisation measurements**; <u>Dirk Wunderlich</u>[1]; Christian Albers[1]; Sylwia Jozwiak[2]; Karina Bora[2]; Ben Wilkes[2]; [1]*Bruker Daltonik GmbH, Bremen, Germany*; [2]*Lonza, Slough, United Kingdom*

TP 030   **Enhancing Host-Cell Protein Detection in Protein Therapeutics Using HILIC Enrichment and Proteomic Analysis**; <u>Qingyi Wang</u>[1]; Thomas R. Slaney[1]; Wei Wu[1]; Richard Ludwig[1]; Li Tao[1]; Anthony Leone[1]; [1]*Bristol-Myers Squibb Company, Pennington, NJ*

TP 031   **Interlaboratory study of an optimised peptide mapping workflow using automated trypsin digestion for monitoring product quality attr**; <u>Silvia Millan Martin</u>[1]; Craig Jakes[1, 2]; Sara Carillo[1]; Tom Buchanan[3]; Marc Guender[4]; Dan Bach Kristensen[5]; Ken Cook[3]; Jonathan Bones[1]; [1]*NIBRT, Dublin, Ireland*; [2]*School of Chemical Engineering and Bioprocessing, University College of Dublin, Dublin, Ireland*; [3]*Thermo Fisher Scientific, Hemel, United Kingdom*; [4]*Thermo Fisher Scientific, reinach, Switzerland*; [5]*Symphogen, Ballerup, Denmark*

TP 032   **A Comprehensive Assessment of Chemical Liabilities in 84 Different SEFL2 IgG1 mAbs**; <u>Chen-Chun Chen</u>[1]; Andrew B. Dykstra[1]; Alex W. Jacobitz[1]; Neelam Khanal[1]; Chris Spahr[1]; Kenneth Walker[1]; Daniel Yoo[1]; Wei Zhang[2]; Yang Yuan Sheng[2]; Nic Angell[1]; Iain D. G. Campuzano[1]; [1]*Amgen Inc., Thousand Oaks, CA*; [2]*Agency for Science, Technology and Research, Singapore, Singapore*

TP 033   **A labeling strategy to improve peptide fragmentation and to distinguish isobaric amino acids by EThcD**; <u>Thierry Le Bihan</u>[1]; Jin Duan[1]; Zac Mc Donald[1]; Xin Xu[1]; Paul Taylor[1]; Qixin Liu[1]; Kathleen Gorospe[1]; Bin Ma[1, 2]; [1]*Rapid Novor Inc, Kitchener*; [2]*University of Waterloo, Waterloo, ON*

TP 034 **Middle down analysis of Herceptin and its biosimilar on a quadrupole-ion trap-Orbitrap mass spectrometer using multiple fragmentations**; Xiaoxi Zhang[1]; Hao Yang[2]; Haichuan Liu[2]; Min Du[3]; [1]*ThermoFisher Scientific, Shanghai, China;* [2]*ThermoFisher Scientific, San Jose, California;* [3]*ThermoFisher Scientific, Massachusetts, Massachusetts*

TP 035 **Site-Specific Conjugation Analysis of an Antibody Drug Conjugate Mimic by Peptide Mapping**; Ken Chanthamontri[1]; Benjamin Cutak[1]; Kevin Ray[1]; [1]*MilliporeSigma, St. Louis, MO*

BIOMARKERS: DISCOVERY I
TP 036-055

TP 036 **Structural Identification of Pentasaccharide Biomarkers for GM1 Gangliosidosis**; Xuntian Jiang[1]; Rohini Sidhu[2]; Pamela Kell[1]; Daniel S Ory[2]; Cynthia J Tifft[3]; Douglas R Martin[4]; Heather L Gray-Edwards[5]; [1]*Washington University in St. Louis, St. Louis, MO;* [2]*Casma Therapeutics, Boston, MA;* [3]*NIH/NHGRI, Bethesda, MD;* [4]*Auburn University, Auburn, AL;* [5]*University of Massachusetts Medical School, Worcester, MA*

TP 037 **Examining effects of increased cytosolic acetyl-CoA levels on Nε-lysine acetylation through proteomic analysis of SLC13A5 and SLC25A1 overexpression**; Hannah Miles[1]; Min Ma[1]; Michael J. Rigby[2]; Nicola Salvatore Orefice[2]; Luigi Puglielli[2]; Lingjun Li[1, 3]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705;* [2]*Department of Medicine and Waisman Center, University of Wisconsin-Madison, Madison, WI 53705;* [3]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*

TP 038 **Evaluation of a Circular Strategy using untargeted LC-HRMS analysis to Discover Biomarkers in Diseases with Long-Tail Distributions of Molecular Mechanisms**; Bertrand Rochat; *Université de Lausanne, Lausanne, Switzerland; Centre Hospitalier Universitaire Vaudois, lausanne, Switzerland*

TP 039 **Finding new colorectal cancer biomarkers through cancer cell secretome characterization**; Emilie-Fleur Gautier[1]; Grégory Leclerc[1]; Aude Le Gall[1]; Jérôme Dupuis[1]; Brian Lockhart[1]; Emmanuel Nony[1]; [1]*Servier Research Institute, Croissy s/Seine, France*

TP 040 **Urinary biomarker discovery and verification in antiretroviral-induced acute kidney injury using SWATH-MS: a retrospective study**; Ireshyn S Govender[1]; Demetra Mavri-Damelin[2]; Previn Naicker[1]; Faheem Seedat[2]; Neil Martinson[2, 3]; Ebrahim Variava[2]; Dalu Mancama[1]; Stoyan Stoychev[1]; [1]*Council for Scientific and Industrial Research, Pretoria, South Africa;* [2]*University of the Witwatersrand, Joahnnesburg, South Africa;* [3]*Johns Hopkins University School of Medicine, Baltimore, Maryland*

TP 042 **Advanced Biomarker Discovery in Imaging Mass Spectrometry Through Interpretable Supervised Machine Learning**; Leonoor Ella Marie Tideman[1]; Lukasz G. Migas[1]; Emilio Rivera[2, 3]; Katerina V. Djambazova[2, 4]; Elizabeth Neumann[2, 3]; Nathan Heath Patterson[2, 3]; Richard M Caprioli[2, 3, 4, 5, 6]; Jeffrey M Spraggins[2, 3, 4]; Raf Van De Plas[1, 2, 3]; [1]*Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands;* [2]*Mass Spectrometry Research Center, Nashville, TN;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [5]*Department of Medicine, Vanderbilt University, Nashville, TN;* [6]*Department of Pharmacology, Vanderbilt University, Nashville, TN*

TP 043 **Investigation on Coagulation Responsive Proteins in Human Serum using Proteomic Techniques**; Abu Hena Mostafa Kamal[1]; Kevin Zhu[1]; Madison Roberts[1]; Gul Nowshad[1]; Lina Abi Mosleh[1]; Mohamad Ammar Ayass[1]; [1]*Ayass BioScience, LLC, Frisco, TX*

TP 044 **Identification and characterization of extracellular matrix proteins enabled by a photo-cleavable surfactant**; Samantha J Knott[1]; Kyle Brown[1]; Harini Josyer[2]; Stanford Mitchell[3]; Austin Carr[2]; David Inman[4]; Suzanne Ponik[4]; Andreas Friedl[5]; Ying Ge[1, 4, 6]; [1]*Department of chemistry, University of Wisconsin Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [3]*Department of Molecular and Cellular Pharmacology, University of Wisconsin-Madison, Madison, WI;* [4]*Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI;* [5]*Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI;* [6]*Director of Mass Spectrometry Human Proteomics Program, University of Wisconsin Madison School of Medicine and Public Health, Madison, WI*

TP 045 **Proteomic Analysis of Human Breast Milk to Reveal Potential Protein Biomarkers for Breast Cancer**; Danielle Whitham[1]; Roshanak Aslebagh[1]; Devika Channaveerappa[1]; Brian Pentecost[2]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; [1]*Clarkson University, Potsdam, NY;* [2]*University of Massachusetts Amherst, Amherst, MA*

TP 046 **Identification and quantification of cholangiocarcinoma (CCA) marker proteins from bile extracellular vesicles for non-invasive diagnosis**; Ayako Kurimoto[1]; Tatsutoshi Inuzuka[1]; Toshiki Ueda[1]; Chisaki Ikeda[2]; Hiroaki Haga[2]; [1]*Miraca Research Institute G.K., Tokyo, Japan;* [2]*Department of Gastroenterology, Faculty of Medicine, Yamagata University, Yamagata, Japan*

TP 047 **Screening of Site-SpecificN-Glycopeptides from Human Serum as Novel Biomarkers for Alzheimer's disease using SteppedHCD-MS/MS**; Lingyun Pan; *UNIVERSITY OF MICHIGAN, ANN ARBOR, MI*

TP 048 **Targeted LC-MS Proteomic Methods to Monitor and Quantify Stromal Conditioning in Cancer from Blood**; Matt Kuruc[1]; Swapan Roy[1]; Wilma Mesker[2]; Rob Tollenaar[2]; [1]*Biotech Support Group LLC, Monmouth Junction, NJ;* [2]*Leiden University Medical Center, Leiden, Netherlands*

TP 049   **Targeted proteomics of cerebrospinal fluid biomarkers in Alzheimer's disease**; Maotian Zhou[1]; Rafi U Haque[1]; Eric B. Dammer[1]; Duc M. Duong[1]; Lingyan Ping[1]; Erik C.B. Johnson[2]; James J. Lah[2]; Allan Levey[2]; Nicholas T Seyfried[2]; *[1]Emory University, atlanta, GA; [2]Emory University, Atlanta, GA*

TP 050   **Identification of Salivary Proteins Responsible for a Peptide Fragment to be used as a Diagnostic Test for Sjögren Syndrome**; Abhijit Roychowdhury[1]; Jasmin De Luna[1, 2]; Earl L White[3]; *[1]MDx BioAnalytical Laboratory, Inc., College Station, TX; [2]Blinn College, Bryan, Texas; [3]MDx BioAnalytical Laboratory, Inc., College Station, Texas*

TP 051   **Pilot Study of Untargeted Urine Metabolomics in Sarcoma Patients Treated with HD-AIM**; Garrett Kinnebrew[1]; Joseph Mcelroy; David Liebner[1]; James L Chen[1]; Ewy Mathe[1]; *[1]The Ohio State University, Columbus, OH*

TP 052   **Proteomic Analysis of BALF using the PASEF method: toward Lung Cancer Biomarker Discovery with 1D LC separation**; Min-Sik Kim[1]; Jun Hyung Lee[1]; Sunghyun Huh[1]; Seo Young Sim[2]; Jinnyoung Choi[3]; Seung Hyeun Lee[2, 4]; *[1]DGIST, Daegu, South Korea; [2]Kyung Hee University, Yongin, South Korea; [3]Bruker Daltonics Korea, Seoul, South Korea; [4]Kyung Hee University School of Medicine, Seoul, South Korea*

TP 053   **Phototoxicity biomarkers for live cell imaging microscopy identified with SWATH mass spectrometry**; Sofia Emmanouela Theodorou; *Institute of Molecular Systems Biology, Department of Biology, ETH Zürich, Zürich, Switzerland*

TP 054   **In-depth proteomics analysis of bovine spermatozoa by tandem mass spectrometry**; Muhammad Imran[1]; Paulos Chumala[1]; Mary Buhr[1]; George S. Katselis[1]; *[1]University of Saskatchewan, Saskatoon, SK*

TP 055   **Plasma Marker Identification of Beta-Cell Injury in Type 2 Diabetes in the GRADE Study, using Isobaric Boosting and Mass Spectrometry**; Antrix Jain[1]; Alexander B. Saltzman[1]; Jong Min Choi; Ruya Liu[2]; Barbara M Brooks-Worrell[3]; Jerry P Palmer[4]; Vijay K Yechoor[2]; Sung Yun Jun[1]; Erica G Hattery[1]; Ashok Balasubramanyam[1]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, TX; [2]University of Pittsburgh, Pittsburgh, PA; [3]University of Washington, Seattle, WA; [4]DVA Puget Sound Health Care System, Seattle, WA*

BIOMARKERS: QUANTITATIVE ANALYSIS I
TP 056-075

TP 056   **Quantitative biomarker to assess teratogenicity of DHODH inhibitors in vivo**; Michael A Pontikos[1]; Christopher Leija[1]; Xiaoyu Wang[1]; Noelle S Williams[1]; Margaret A Phillips[1]; *[1]University of Texas Southwestern Medical Center, Dallas, TX*

TP 057   **Proteomic Biomarkers of Multiparametric Magnetic Resonance Imaging Visibility in Prostate Cancer**; Amanda Khoo[1]; Taylor Y. Sadun[2]; Vladimir Ignatchenko[3]; Lydia Y. Liu[1]; Aydin Pooli[2]; Katie Houlahan[1]; Steven S. Raman[2]; Anthony E. Sisk Jr.[2]; Paul C. Boutros[2]; Robert E. Reiter[2]; Thomas Kislinger[1, 3]; *[1]University of Toronto, Toronto, ON; [2]Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA; [3]Princess Margaret Cancer Centre, Toronto, ON*

TP 058   **Challenges in Protein Tyrosine Phosphorylation Measurement by LC-MS/MS: Assay Optimization Strategies to Quantify Site-Specific Phosphorylated BTKs for Clinical Development**; Naiyu Zheng[1]; Kristin Taylor[1]; Rong Liu[1]; Scott Robotham[1]; Rasa Santockyte[1]; Lihong Cheng[1]; Yi Luo[1]; Yan J. Zhang[1]; Renuka Pillutla[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

TP 059   **A Simple, Rapid Method for Simultaneously Quantitative Analysis of Glutathione and Glutathione Disulfide in Rodent Biofluid and Tissue Samples**; Yunhui Zhang; *Charles River Laboratories, Worcester, MA*

TP 061   **A Methylated Protein Biomarker of Target Engagement in Blood and Tumors: From Proteomic Screen to Clinical Assay**; Timothy Sikorski[1]; Paul Noto[1]; Francesca Zappacosta[1]; Craig Wagner[1]; Rocio Montes De Oca[1]; Matthew Szapacs[1]; Roland S Annan[1]; Yan Liu[1]; Charles Mchugh[1]; Steven Piccoli[1]; Caretha Creasy[1]; *[1]GlaxoSmithKline, Collegeville, PA*

TP 062   **A Multiomic Evaluation the Effects of Exercise and Menopause on Cognition in Alzheimer's Disease Mouse Models**; Kendra J. Adams[1]; Janai Williams[1]; Lisa St. John-Williams[1]; Sarah Hiles[1]; Carol A. Colton[1]; M. Arthur Moseley[1]; Christina L. Williams[1]; J. Will Thompson[1]; *[1]Duke University, Durham, NC*

TP 063   **A Sensitive Immuno-MRM Assay for Quantifying PTEN to Allow Better Stratification of Breast Cancer Patients**; Sahar Ibrahim[1]; Naciba Benlimame[2]; Adriana Aguilar-Mahecha[3]; Alan Spatz[4]; Mark Basik[5, 6]; Gerald Batist[5, 6]; Constance A. Sobsey[1]; Christoph H. Borchers[1, 6, 7]; René Zahedi[1]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [2]Pathology Research Department, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [3]Cancer Genomics and Translational Research Laboratory, Segal Cancer Center, Lady Davis Institute for Medical Research, Sir Mortimer B. Davis Jewish General Hospital, Montreal, QC; [4]Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; [5]Segal Cancer Center, Lady Davis Institute for Medical Research, Sir Mortimer B. Davis Jewish General Hospital, McGill University, Montreal, QC; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [7]Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

TP 064 **Application of Chemical Derivatization in LC-MS Analysis to Support PK/PD and Biomarker Studies**; Fangbiao Li[1]; Bang-lin Wan[1]; Guangping Bi[1]; Rena Zhang[1]; Daniel S Spellman[1]; [1]*Merck & Co., Inc., West Point, PA*

TP 065 **Targeted quantitative proteomic approach to develop blood diagnostic test of mental illnesses by Liquid Chromatography and Tandem Mass Spectrometry (LC-MS/MS)**; Jihyeon Lee[1]; Areum Sohn[1]; Sangjin Rhee[2]; Yongmin Ahn[2]; Youngsoo Kim[1, 3]; [1]*Department of Biomedical Sciences, Seoul National University, Seoul, South Korea;* [2]*Department of Neuropsychiatry, Seoul National University Hospital, Seoul, South Korea;* [3]*Interdisciplinary Program of Bioengineering, Seoul National University College of Engineering, Seoul, South Korea*

TP 066 **Mass Spectrometry Analysis of Protein Expression in Honey Bees**; Kermit K. Murray[1]; Chao Dong[1]; Fabrizio Donnarumma[1]; Vincent A Ricigliano[2]; Touradj Solouki[3]; Luke Richardson[3]; [1]*Louisiana State University, Baton Rouge, LA;* [2]*USDA-ARS Honey Bee Breeding, Genetics, and Physiology Laboratory, Baton Rouge, LA;* [3]*Baylor University, Waco, TX*

TP 067 **Efficient tandem mass spectrometry method for the analysis of methylmalonic acid in urine**; Tristan Martineau[1]; Michel Boutin[1]; Audrey Perreault[2]; Pierrette Gaudreau[3]; Nancy Presse[1]; Christiane Auray-Blais[1]; [1]*Université de Sherbrooke, Sherbrooke, QC;* [2]*CIUSSS-de-l'Estrie-CHUS, Sherbrooke, QC;* [3]*Université de Montréal, Montréal, QC*

TP 068 **A Quantitative study of potential blood biomarker for Alzheimer's Disease by Targeted Mass Spectrometry**; Yeongshin Kim[1]; Jaenyeon Kim[1]; Joonho Park[1]; Minsoo Son[1]; Youngsoo Kim[1, 2, 3]; [1]*Interdisciplinary Program of Bioengineering, Seoul National University College of Engineering, Seoul, South Korea;* [2]*Department of Biomedical Sciences, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea;* [3]*Department of Biomedical Engineering, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea*

TP 069 **Urinary isomeric dimethylarginine ratio and its plausible diagnostic value for diabetic nephropathy**; Dharmeshkumar Parmar[1, 2]; Nivedita Bhattacharya[1, 2]; Shanthini Kannan[3]; Sangeetha Vadivel[3]; Prabhakar Sripadi[4]; Gokulakrishnan Kuppan[3]; Venkateswarlu Panchagnula[2, 5]; [1]*CSIR-National Chemical Laboratory, Pune, India, Pune, India;* [2]*Academy of Scientific and Innovative Research (AcSIR), Pune, India;* [3]*Madras Diabetes Research Foundation, Chennai, India;* [4]*CSIR-Indian Institute of Chemical Technology, Hyderabad, India;* [5]*National Chemical Laboratory, Pune, India, Pune, India*

TP 070 **A Standardized Workflow for Developing Protein Immunoprecipitation Assays to Support Clinical Endpoints**; Brendan Tierney[1]; Ying Zhang[1]; Kyle Wald[1]; Matthew Blatnik[1]; [1]*Pfizer Worldwide Research and Development, Groton, CT*

TP 071 **Online 2-dimensional Strong Cation Exchange/Reverse-phase LCMS Analysis for the Cataloging of Proteins in Human Heart**; Matthew Mazur[1]; Bogdan Sleczka[1]; Petia Shipkova[1]; Timothy Olah[1]; [1]*Bristol-Myers Squibb Company, Princeton, NJ*

TP 072 **Serum glycoprotein markers in non-alcoholic steatohepatitis (NASH) and hepatocellular carcinoma (HCC)**; Prasanna Ramachandran[1]; Gege Xu[1]; Ling Shen[1]; Daniel Serie[1]; [1]*InterVenn Biosciences, South San Francisco, CA*

TP 073 **Evaluation of Matrix Effects on an Immunoaffinity LC-MS Method for the Quantitation of IGF1 in Human Serum**; Kevin Ray[1]; Pegah Jalili[1]; Judy Cao[1]; Uma Sreenivasan[2]; [1]*MilliporeSigma, St. Louis, MO;* [2]*MilliporeSigma, Round Rock, TX*

TP 074 **Quantitative Analysis of N-Glycans in Human Blood Serum Derived from Patients with Moderate to Severe Traumatic Brain Injury using LC-MS/MS**; Kaitlyn B Donohoo[1]; Mona Goli[1]; Byeong Gwan Cho[1]; Alireza Banazadeh[1]; Firas Kobaissy[2]; Ryan Morgan[1]; Jingfu Zhao[1]; Endre Czeiter[3, 4, 5]; Krisztina Amrein[3, 4, 5]; Andras Buki[3, 4, 5]; Sakshi Gautam[1]; Wenjing Peng[1]; Stefania Mondello[6, 7]; Yehia Mechref[1, 8]; [1]*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas;* [2]*Department of Psychiatry and Neuroscience, McKnight Brain Institute, University of Florida, Gainesville, Florida;* [3]*Department of Neurosurgery, University of Pecs, Pecs, Hungary;* [4]*Janos Szentagothai Research Centre, University of Pecs, Pecs, Hungary;* [5]*MTA-PTE Clinical Neuroscience MR Research Group, Pecs, Hungary;* [6]*Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy;* [7]*Oasi Research Institute-IRCCS, Troina, Italy;* [8]*Center for Biotechnology and Genomics, Texas Tech University, Lubbock, Texas*

TP 075 **Commercial LC-MS/MS assay for accurate quantification of Hepcidin in the context of iron homeostasis and inflammation processes**; Fabian Simon[1]; Ayseguel Aksan[2]; Florian Bonn[1]; Anne Arnold[1]; Juergen Stein[2]; Franz Paul Armbruster[1]; [1]*Immundiagnostik AG, Bensheim, Germany;* [2]*Interdisciplinary Crohn Colitis Center Rhein-Main, Frankfurt, Rhein-Main, Germany*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING I
TP 076-094

TP 076 **Fluorinated Acyl-transfer Reagent Efficaciously Benzoylates Nucleophilic Residues for Application in Covalent-labeling Mass Spectrometry: A New Validation Workflow**; Austin B. Moyle[1]; Ming Cheng[1]; Nicole D. Wagner[1]; Michael L. Gross[1]; [1]*Washington University, St. Louis, St. Louis, MO*

TP 077 **Developing Quantitative Methods to Analyze Disulfide Bond Shuffling During Protein Aggregation using Covalent Labeling-Mass Spectrometry**; M. Cyndell Gracieux[1]; Bea Sewell[1]; Michael B. Goshe[1]; [1]*North Carolina State University, Raleigh, NC*

TP 078 **Diethylpyrocarbonate Modified Histidine Isomers Reveal Higher Resolution Protein Structural Information**; Xiao Pan[1]; Tianying Liu[2]; Patanachai Kong Limpikirati[2]; Richard W Vachet[2]; [1]*University of Massachusetts-Amherst, Amherst, MA; [2]University of Massachusetts Amherst, Amherst, MA*

TP 081 **Spheroid-FPOP, an Extension of In-Cell Fast Photochemical Oxidation of Proteins (IC-FPOP)**; Raquel Shortt[1]; Yijia Wang[2]; Amanda B. Hummon[2]; Lisa Jones[1]; [1]*University of Maryland Balitmore, Baltimore, MD; [2]Department of Chemistry and Biochemistry, Ohio State University, Ohio Columbus, Ohio*

TP 082 **Crosslinked peptide support in Skyline**; Nicholas Shulman[1]; Alex Zelter[1]; Michael J MacCoss[1]; Brendan Maclean[1]; [1]*Department of Genome Sciences, University of Washington, Seattle, WA*

TP 083 **Combined UV Laser Ablation and Photochemical Oxidation of Proteins for Mass Spectrometry**; Oluwatosin A Ogundairo[1]; Fabrizio Donnarumma[1]; Kermit K Murray[1]; [1]*Louisiana State University, Baton Rouge, LA*

TP 084 **Development of a Thiol Exchange- and Mass Spectrometry-Based Technique for the Evaluation of Protein Folding Stabilities**; Aurora F. Cabrera[1]; Terrence G. Oas[2]; Michael C. Fitzgerald[1]; [1]*Department of Chemistry, Duke University, Durham, NC; [2]Department of Biochemistry, Duke University Medical Center, Durham, NC*

TP 085 **Simple Cross-Linking/Mass Spectrometry Workflows for Studying System-Wide Protein Interactions**; Claudio Iacobucci[1]; Michael Goetze[1]; Christian H Ihling[1]; Andrea Sinz[1]; [1]*Martin Luther University Halle, Halle, Germany*

TP 086 **MALDI Analysis for Protein Footprinting**; Jerry Jiang[1]; Michael L. Gross[2]; [1]*Washington University at St. Louis, St. Louis, MO; [2]Washington University in St.Louis, St.Louis, Missouri*

TP 087 **Can Overlabeling with DEPC Give Correct Protein Structural Information?**; Zachary J Kirsch[1]; Richard W Vachet[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

TP 088 **Use of multiple ion fragmentation methods to identify protein cross-links and facilitate comparison of data interpretation algorithms**; Bingqing Zhao[1]; Colin P. Reilly[1]; James P. Reilly[1]; [1]*Indiana University, Bloomington, IN*

TP 089 **OpenPepXL: An open-source tool for sensitive identification of cross-linked peptides in XL-MS**; Eugen Netz[1]; Tjeerd MH Dijkstra[2]; Timo Sachsenberg[3]; Oliver Kohlbacher[1, 3, 4, 5]; [1]*Max Planck Institute for Developmental Biology, Tübingen, Germany; [2]Max Planck Institute for Developmental Biology, Tuebingen, Germany; [3]Applied Bioinformatics, Tübingen, Germany; [4]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [5]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

TP 090 **How to prepare samples for affinity purification combined with crosslinking mass spectrometry (AP-XLMS)**; Yan Hao[1]; Ying Zhang[2]; Zhihui Wen[2]; Charles A.S. Banks[2]; Michael P. Washburn[2, 3]; Laurence Florens[2]; [1]*Stowers Institute for Medical Research, Kansas city, MO; [2]Stowers Institute for Medical Research, Kansas City, MO; [3]Department of Pathology and Laboratory Medicine, University of Kansas Medical Center, Kansas City, KS*

TP 091 **MS-Scout: An all-rounded environment for regular and cleavable cross-linking mass spectrometry**; Milan Avila Clasen[1]; Diogo Borges Lima[2]; Louise Ulrich Kurt[3]; Marlon Dias Mariano Dos Santos[3]; Fabio Cesar Gozzo[4]; Paulo Costa Carvalho[3]; [1]*Fiocruz - PR, Carlos Chagas Institute, Curitiba, Brazil; [2]Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; [3]Fiocruz - PR, Carlos Chagas Institute, Curitiba, Brazil; [4]University of Campinas, Campinas, Brazil*

TP 092 **Optimization of LCMS acquisition settings for detection of crosslinked peptides**; Ying Zhang[1]; Zhihui Wen[1]; Edward A Partlow[2]; Gunther Hollopeter[2]; Laurence Florens[1]; Michael P. Washburn[1, 3]; [1]*Stowers Institute for Medical Research, Kansas City, MO; [2]Department of Molecular Medicine, College of Veterinary Medicine, Cornell University, Ithaca, NY 14853; [3]Department of Pathology and Laboratory Medicine, University of Kansas Medical Center,, Kansas City, KS*

TP 093 **Minimizing Search Space Inflation Associated with False Discovery Rate Estimation in Cross-Linking Mass Spectrometry Database Searches**; D. Alex Crowder[1, 2]; Vladimir Sarpe[1]; Daniel S. Ziemianowicz[1, 2]; Atefeh Rafiei[3]; David C. Schriemer[1, 2, 3]; [1]*Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; [2]Robson DNA Science Centre, Arnie Charbonneau Cancer Institute, University of Calgary, Calgary, AB; [3]Department of Chemistry, University of Calgary, Calgary, AB*

TP 094 **A crosslinking – mass spectrometry based multi-level integrative modeling approach to resolve the microtubule-doublecortin interaction**; Atefeh Rafiei[1]; David C. Schriemer[1]; [1]*University of Calgary, Calgary, AB*

CARBOHYDRATES II
TP 095-114

TP 095   **Comprehensive Profiling of O-linked Glycans in Bovine Submaxillary Mucin**; Yang Tang[1]; Juan Wei[2]; Catherine E. Costello[1, 2]; Cheng Lin[2]; [1]*Boston University, Boston, MA;* [2]*Boston University School of Medicine, Boston, MA*

TP 096   **Progress towards a clinically viable glycomics assay for uromodulin, a protein exclusively produced in kidneys**; Milani Wijeweera Patabandige[1]; Eden P Go[1]; Heather Desaire[1]; [1]*University of Kansas, Lawrence, Kansas (KS)*

TP 097   **Glycomic Mapping of Maize Carbohydrates Using a High-Throughput LC-MS-Based Platform**; Garret Couture[1]; Thai-Thanh T Vo[1]; Juan J Castillo[1]; Nikita Bacalzo[1]; Carlito B Lebrilla[1]; [1]*University of California, Davis, Davis, CA*

TP 098   **Parallel Reaction Monitoring of Permethylated N-glycans Probing Different Isomer Fragmentations and Improving Sensitivity**; Andrew Cho[1]; Sakshi Gautam[1]; Alireza Banazadeh[1]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX*

TP 099   **Supplementing Liquid Chromatography-Mass Spectrometry with Nuclear Magnetic Resonance for In-Depth Structural Determination of Oligosaccharides and Polysaccharides**; Siyu (Cathy) Chen[1]; Juan J. Castillo[1]; Yixuan (Axe) Xie[1]; Carlito B. Lebrilla[1]; [1]*University of California, Davis, Davis, CA*

TP 100   **Identification and quantitation of polysaccharides in plants and dietary fibers**; Nikita Bacalzo[1]; Juan J Castillo[1]; Garret Couture[1]; Eshani Nandita[1]; Carlito B Lebrilla[1]; [1]*UC Davis, Davis, CA*

TP 101   **Sequencing and Structural Characterization of Carbohydrate Oligosaccharides using Tandem Trapped Ion Mobility Spectrometry–Mass Spectrometry (TIMS/TIMS-MS)**; Jusung Lee[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

TP 102   **Discovering bioactive oligosaccharides in wine byproducts through quadrupole time-of-flight and triple quadrupole mass spectrometry**; Amanda JG Sinrod[1]; Mrittika Bhattacharya[1]; Juan J. Castillo[1]; Daniela Barile[1]; [1]*University of California, Davis, Davis, CA*

TP 103   **Comparison between MicroPillar Array Column（µPAC™) and C18-packed column for N- and O-linked glycopeptides profiling using LC-MS/MS**; Jieqiang Zhong[1]; Yifan Huang[1]; Yehia Mechref[1]; [1]*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*

TP 104   **An in-depth Comparison of the Pediatric and Adult Urinary Glycomes**; Haiying Li[1]; Viral Patel[1]; Shannon E Dimartino[1]; John W Froehlich[1]; Richard S Lee[1]; [1]*Boston children's hospital, Boston, MA*

TP 105   **New free oligosaccharides found in bovine milk by new MS method potentially lead to discovery of new biosynthesis pathway**; Weichien Weng[1]; Chi-Kung Ni[1]; Shih-Pei Huang[1]; Hsu Chen Hsu[1]; [1]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City, Taiwan*

TP 106   **Multivariate Analysis of Tandem Mass Spectrometry Data Distinguishes Epimeric Glycosaminoglycans**; Jandi Kim[1]; Lauren E. Pepi[1]; Fuming Zhang[2]; Robert J. Linhardt[2]; I. Jonathan Amster[1]; [1]*University of Georgia, Athens, GA;* [2]*Rensselaer Polytechnic Institute, Troy, NY*

TP 107   **Serum Glycomic Profiling of Patients with Primary Restless Legs Syndrome (RLS) using LC-MS/MS**; Xue Dong[1]; Stefania Mondello[2, 3]; Firas Kobeissy[4]; Raffaele Ferri[3]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX;* [2]*University of Messina, Messina, Italy;* [3]*Oasi Research Institute-IRCCS, Troina, Italy;* [4]*American University of Beirut, Beirut, Lebanon*

TP 108   **Quantitation and Characterization of Glycans via Free Radical Isotopic/Isobaric Tags**; Rayan M Murtada[1]; Jinshan Gao[1]; [1]*Montclair State University, Montclair, NJ*

TP 109   **On slide tissue digestion coupled glycomics and proteomics analysis of myelinated versusnon-myelinated regions of human brain tissue.**; Manveen K Sethi[1]; Oliver King[2]; Harry Pantazopoulos[2]; Sabina Berretta[2]; Joseph Zaia[1]; [1]*Boston University School of Medicine, Boston, MA;* [2]*Harvard Medical School, Boston, MA*

TP 110   **Permethylated N-glycan Profiling using Micropillar Arrays Columns (µPACTM)-LC-MS**; Peilin Jiang[1]; Byeong Gwan Cho[1]; Sakshi Gautam[1]; Mona Goli[1]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX*

TP 111   **Electron Induced Dissociation of Singly-Charged Peptides and Glycans in Modified Q-TOF and QE Orbitrap Mass Spectrometers**; Diana M. Oppenheimer[1]; Yury V. Vasil'ev[1, 2]; Michael C. Hare[1]; Valery G. Voinov[1, 2]; Joseph S. Beckman[1, 2]; [1]*e-MSion, Inc., Corvallis, OR;* [2]*Oregon State University, Corvallis, OR*

TP 112   **Capillary Zone Electrophoresis-Tandem Mass Spectrometry Analysis of Long Chain Chondroitin Sulfate / Dermatan Sulfate and Bikunin**; Yiqing Zhang[1]; Gina Renois Predelus[1]; Morgan Stickney[1]; Patience Sanderson[1]; Jon Amster[1]; [1]*University of Georgia, Athens, GA*

TP 113   **Capillary Zone Electrophoresis Negative Electron Transfer Dissociation Mass Spectrometry (CZE-NETD-MS) Analysis of Protein Pull-Down Glycosaminoglycans**; Gina Renois Predelus[1]; Jon Amster[1]; [1]*University of Georgia, Athens, GA*

TP 114   **Relative Quantitation of HeLa Cell N-Glycans Using Deuterium Oxide Labeling for Global Omics Relative Quantification(DOLGOReQ)**; Jonghyun Kim[1]; Jua Lee[2, 3]; Dongtan Yin[2, 3]; Hyun Joo An[2, 3]; Tae-Young Kim[1]; [1]*Gwangju Institute of Science & Technology, Gwangju, South Korea;* [2]*Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea;* [3]*Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea*

CLINICAL ANALYSIS I
TP 115-134

TP 115   **Development, Validation and Implementation of Patient-centric Volumetric Absorptive Microsampling-LC-MS/MS Assays for the Analysis of Anti-bacterial Drugs in Pediatric Subjects**; Ganesh Moorthy[1]; Christina Vedar[1]; Nicole R Zane[1]; Kevin J Downes[1]; Athena F Zuppa[1]; [1]*Children's Hospital of Philadelphia, Philadelphia, PA*

TP 116   **LC-MS/MS-based enzyme assay for lysosomal storage disorders using dried blood spots**; Ryuichi Mashima[1]; Mari Ohira[1]; Torayuki Okuyama[1]; [1]*National Center for Child Health and Development, Setagaya-Ku, Japan*

TP 117   **Characterization of Clinically Unidentified Hemoglobin Variants by 21 Tesla Fourier Transform Ion Cyclotron Resonance Tandem Mass Spectrometry**; Yuan Lin[1, 2]; Lidong He[1]; Lissa C. Anderson[2]; Archana M. Agarwa[3, 4]; Alan L. Rockwood[1, 3, 5]; Chad R. Weisbrod[2]; Christopher L. Hendrickson[2]; Alan G. Marshall[1, 2]; [1]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL;* [2]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [3]*University of Utah Health, Salt Lake City, UT;* [4]*ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT;* [5]*Rockwood Scientific Consulting, Salt Lake City, UT*

TP 118   **Comparison of Whole Blood and Precipitated Blood for the Quantitation of Drugs of Abuse Using PaperSpray**; Katherine Walker[1]; Yu Zhu[1]; Neloni Wijeratne[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

TP 119   **Evaluation of automated quantitative analysis of the doubly charged glycatedβ-hemoglobin by MALDI-TOF MS**; Dennis JA Van Den Heuvel[1]; Andreas Schnapp[2]; Johan Scholtens[3]; [1]*Shimadzu Benelux, 's-Hertogenbosch, Netherlands;* [2]*Shimadzu Europa GmbH, Duisburg, Germany;* [3]*Shimadzu Benelux, 's-Hertogenbosch, Netherlands*

TP 120   **Fully automated LC-MS/MS method to assess DPD deficiency in Cancer treatment with 5-FU**; Sascha Rexroth[1]; Doriane Toinon[2]; Tiphaine Robin[3, 4]; Stéphane Moreau[1]; Franck Saint-Marcoux[4]; [1]*Shimadzu Europa GmbH, Duisburg, Germany;* [2]*Shimadzu Corporation, Kyoto, Japan;* [3]*Shimadzu France, Paris, France;* [4]*CHU Limoges, Limoges, France*

TP 121   **Development and Application of HPLC with Data-Dependent Ion-Trap MS2 for Clinical Toxicology Screening of 38 Drugs and Metabolites** ; Nicholas Laude[1]; Caitlyn Kanzian[1]; Kenneth Funk[1]; William Edgemond[1]; [1]*Genotox Laboratories, Austin, TX*

TP 122   **Monitoring of embryonic stem cell differentiation trajectories by intact cell mass spectrometry**; Petr Vaňhara[1, 2]; Andreas Schnapp[3]; Lukáš Moráň[1, 2]; Lukáš Pečinka[4]; Hana Kotasová[1, 2]; Vendula Pelková[2]; Josef Havel[1, 4]; Aleš Hampl[1, 2]; [1]*International Clinical Research Center, St. Anne's University Hospital Brno, Brno, Czech Republic;* [2]*Faculty of Medicine, Masaryk University, Brno, Czech Republic;* [3]*Shimadzu Europa GmbH, Duisburg, Germany;* [4]*Faculty of Science, Masaryk University, Brno, Czech Republic*

TP 123   **Quantification of Free Fatty Acid Isomers in Untreated Clinical Samples via Thread-based Atmospheric Pressure Chemical Ionization**; Devin Swiner[1]; Hannah Osae[1]; George R. Durisek, Iii[1]; Abraham K. Badu-Tawiah[1]; [1]*The Ohio State University, Columbus, OH*

TP 124   **Rapid Intraoperative Detection of Isocitrate Dehydrogenase Mutations in Human Gliomas using a Miniature Mass Spectrometer**; Hannah Marie Brown[1]; Fan Pu[1]; Mahua Dey[2]; James Miller[2]; Mitesh V. Shah[2]; Scott A. Shapiro[2]; Zheng Ouyang[1, 3]; Aaron A. Cohen-Gadol[2]; R. Graham Cooks[1]; [1]*Department of Chemistry and Bindley Biosciences Center, Purdue University, West Lafayette, IN;* [2]*Department of Neurological Surgery, Indiana University School of Medicine, Indianapolis, Indiana;* [3]*Department of Precision Instrument, Tsinghua University, Beijing, China*

TP 125   **How to solve the disappearing methionine puzzle in new born screening?**; Konrad Piotr Kowalski[1]; Tomasz Bieńkowski[2, 3]; Anna Kołodyńska-Goworek[2]; Katrzyna Połeć-Pawlak[2, 4]; Anna Czyż[4]; [1]*Masdiag Sp. z o.o., Warszawa, Poland;* [2]*Masdiag Sp. z o.o., Warszawa, Poland;* [3]*MS Ekspert Sp. z o.o., Gdańsk, Poland;* [4]*Warsaw University of Technology, Warszawa, Poland*

TP 126   **MALDI-TOF IP-MS quantification of plasma amyloid peptides in Alzheimer's disease**; Jerome Vialaret[1]; Jana Kindermans[1]; Sylvain Lehmann[1]; Audrey Gabelle[2]; Christophe Hirtz[1]; [1]*IRMB, Univ Montpellier, INSERM, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France;* [2]*Montpellier university, CHU Montpellier, CMRR, Montpellier, France*

TP 127   **Validation of Metabolic Analysis by Desorption Electrospray Ionization Mass Spectrometry Imaging for Preoperative Diagnosis of Thyroid Nodules**; Rachel J. DeHoog[1]; Monica Lin[1]; Jialing Zhang[1]; John Lin[1]; Kirtan Brahmbhatt[2]; Wendong Yu[2]; Robert Tibshirani[3]; James Suliburk[2]; Livia S Eberlin[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*Baylor College of Medicine, Houston, TX;* [3]*Stanford University, Stanford, CA*

TP 128   **Use of Superoxide Adduct in LDTD with Differential Mobility to Improve Selectivity for 25-OH-Vitamin D2/D3 Analysis in 9 Seconds**; Serge Auger[1]; Pierre Picard[1]; Jean Lacoursière[1]; [1]*Phytronix Technologies, Quebec, QC*

TP 129   **Determination of sex hormones in human serum and plasma using a LC/TQ medical device**; Suparna Mundodi[1]; Xiaoli Dong[1]; [1]*Agilent Technologies, Santa Clara, CA*

TP 130   **Deep, reproducible and high-throughput FFPE analyses: moving toward large-scale clinical omics applications**; Matthew Willetts[1]; Christopher Swift[2]; John P Wilson[3]; Shourjo Ghose[2]; [1]*Bruker, Billerica, MA;* [2]*Bruker Daltonics, Billerica, MA;* [3]*ProtiFi, LLC, Farmingdale, NY*

TP 131   **Steroid Conjugates: an aid for a comprehensive insight of endocrine health**; Ahmed Najar[1]; Melissa Bennett[1]; George Gillson[1]; [1]*LifeLabs, Calgary, AB*

TP 132   **Intraoperative analysis of human breast and lymph node tissues during lumpectomy and mastectomy surgeries using the MasSpec Pen Technology**; Kyana Y Garza[1]; Jialing Zhang[1]; Marta Sans[1]; Rachel J DeHoog[1]; Mary King[1]; Clara L Feider[1]; Alena Bensussan[1]; Michael F Keating[1]; John Lin[1]; Stacey A Carter[2]; Alastair Thompson[2]; Elizabeth Bonefas[2]; Chandandeep Nagi[2]; Chris Pirko[2]; Kirtan Brahmbhatt[2]; James Suliburk[2]; Livia S Eberlin[1]; [1]*University of Texas, Austin, TX;* [2]*Baylor College of Medicine, Houston, TX*

TP 133   **Liquid Chromatography-Mass Spectrometry Determination of Atorvastatin in Eye Vitreous Humor of Diabetic Patients**; Kingsley Donkor[1]; Taran Main[1]; Colten Wendel[2]; Zhi Chao Guo[1]; [1]*Thompson Rivers University, Kamloops, BC;* [2]*St. Paul's Hospital, Vancouver, BC*

TP 134   **Thin film molecularly imprinted polymers (MIPs) for selective and high throughput analysis of biological samples**; Fereshteh Shahhoseini[1]; Evan A. Langille[2]; Ali Azizi[2]; Carlos A. Bazan[2]; Christina Bottaro[2]; [1]*Memorial University of Newfoundland, St. John's, NL;* [2]*Memorial University, St. John's, NL*

CORPORATE POSTERS II
TP 135-137

TP 135   **Bruker at ASMS 2020: MALDI II for dramatic sensitivity improvements in SpatialOMx workflows, Bruker Daltonics**

TP 136   **Analytical Intelligence in the Digital Age of Mass Spectrometry, Shimadzu Scientific Instruments**

TP 137   **Orbitrap Exploris Mass Spectrometry, Thermo Fisher Scientific**

DRUG DISCOVERY/DMPK/ADME II
TP 138-149

TP 138   **Plasmodium chaperonin TCP-1 identified as target of antihistamine clemastine using energetic-based proteomics studies**; Baiyi Quan[1]; Kuan-Yi Lu[1, 2]; Kayla R. Sylvester[2]; Tamanna Srivastava[1]; Michael C. Fitzgerald[1]; Emily R. Derbyshire[1, 2]; [1]*Department of Chemistry, Duke University, Durham, NC;* [2]*Department of Molecular Genetics and Microbiology, School of Medicine, Duke University, Durham, NC*

TP 139   **The fastest ESI-MS: Mass spectrometry analysis up to six samples per second by acoustic ejection**; Tim T Häbe[1]; Frank Runge[1]; Chang Liu[2]; Tom R Covey[2]; Andreas Harald Luippold[1]; [1]*Boehringer Ingelheim, Drug Discovery Sciences, Biberach an der Riss, Germany;* [2]*SCIEX, Concord, ontario*

TP 140   **Distinct pharmacokinetics and tissue distribution study of four structure similar epidermal growth factor receptor inhibitors using quantitation LC-MS/MS**; Lu Wang[1]; Miao He[1]; Bo Wen[1]; Manjunath Pai[1]; Hebao Yuan[1]; Duxin Sun[1]; [1]*University of Michigan, Ann Arbor, MI*

TP 141   **Development of a clinically relevant dosing (CRD) approach in mice for studying acquisition of antibiotic resistance**; Xiaoyu Wang[1]; Erika Serrano Diaz[1]; Laura Coughlin[1]; Marguerite Monogue[1]; Andrew Y. Koh[1]; Erdal Toprak[1]; Noelle S Williams[1]; [1]*UT Southwestern Medical Center, Dallas, TX*

TP 142   **Trapping of Reactive Acyl Glucuronides by a Protein Surrogate as a Tool for the Assessment of Potential Idiosyncratic Toxicities**; Jian Yu[1]; Heng Keang Lim[2]; Rhys Salter[1]; Kaushik Mitra[1]; [1]*Drug Metabolism and Pharmacokinetics, Discovery Sciences, Janssen Pharmaceutical companies of Johnson & Johnson, Springhouse, PA;* [2]*Drug Metabolism and Pharmacokinetics, Discovery Sciences, Janssen Pharmaceutical companies of Johnson & Johnson, Springhouse, PA*

TP 143   **Analysis of Biochemical Reactions at 1 Hz using the Echo-Mass Spectrometer: Accelerated Hit Triage for a Lipid Metabolizing Enzyme**; Xiujuan Wen[1]; Kiersten Tovar[1]; Lucien Ghislain[2]; Chang Liu[3]; Kenneth Ellsworth[1]; Mary Jo Wildey[1]; David G Mclaren[1]; [1]*Merck & Co., Kenilworth, NJ;* [2]*Beckman Coulter Life Sciences, San Jose, CA;* [3]*SCIEX, Concord, ontario*

TP 144   **Hepatocyte Spheroids as a Viable in vitro Model for Recapitulation of Complex in vivo Metabolism Pathways of Loratadine in Humans**; <u>Silvi Chacko</u>[1]; Van T Ly[2]; Lisa J. Christopher[2]; Jinping Gan[2]; [1]*Bristol-Myers Squibb, Princeton, NJ;* [2]*Bristol-Myers Squibb Company, Princeton, NJ*

TP 145   **Identification and Characterization of Non-Covalent Small Molecule Binders of mRNA and Proteins using Affinity Selection-Mass Spectrometry (ASMS)**; <u>Can Ozbal</u>[1]; William Albino Lamarr[1]; Ian Mckenna; Arrin Katz[1]; [1]*PureHoney Technologies, Inc., Billerica, MA*

TP 146   **Intact Protein Analysis Enables Pharmacokinetic/Pharmacodynamic Profiling of Covalent Drug Candidates**; <u>Md Amin Hossain</u>[1]; Rutali R. Brahme[1]; Jakal Amin[1]; Durgalakshmi Sivasankar[1]; Tanvi Gawde[1]; Aparna C. Aparna C. Ponmudiyan[1]; Daniel P. Donnelly[1]; Jared R. Auclair[1]; Brandon Miller[1]; Roman Manetsch[1]; David J. Greenblatt[2]; Jeffrey N. Agar[1]; [1]*Northeastern University, Boston, MA;* [2]*Tufts University, Boston, Massachusetts*

TP 147   **Mass Spectrometry Applied for Automated Phenotyping of Clinical Trial Populations – Approach Extended to a CYP2C8 Specific Assay**; <u>Thomas Lloyd</u>[1]; Eduardo E. Lopez[1]; [1]*Worldwide Clinical Trials, Austin, TX*

TP 148   **Mass Spectral Characterization of Bilirubin by Electrospray Ionization, H/D Exchange, and Multiple Stage Mass Spectrometry**; <u>Stephen U Bowlin</u>[1]; Amin Kamel[1]; [1]*Takeda California, San Diego, CA*

TP 149   **A High-Throughput Hepatocyte Stability Assay for Compound Screening in Early Drug Discovery using a Semi-automated Pipetting System**; <u>Catalina Suarez</u>[1]; Qi Wu[1]; Yongying Jiang[1]; [1]*UT MD Anderson Cancer Center, Houston, TX*

ENVIRONMENTAL: GENERAL I
TP 150-171

TP 150   **Determination of Haloacetic Acids, Bromate, and Dalapon in Drinking Water Using Ion Chromatography Coupled to High-Resolution Accurate-Mass (IC-HRAM) Mass Spectrometry**; <u>Beibei Huang</u>[1]; Jeffrey Rohrer[1]; [1]*Thermo Fisher Scientific, Sunnyvale*

TP 151   **FT-ICR MS Reveals the Structural Dependence of Emerging and Recalcitrant Contaminants Generated from the Widespread Use of Natural Products**; <u>Taylor J. Glattke</u>[1, 2]; Martha L. Chacón-Patiño[1]; Sydney F. Niles[1, 2]; Christopher L. Hendrickson[1, 2]; Alan G. Marshall[1, 2]; Ryan P. Rodgers[1, 2]; [1]*FSU-National High Magnetic Field Laboratory, Tallahassee, FL;* [2]*Florida State University, Tallahassee, FL*

TP 152   **Rapid and Sensitive Analysis of Perfluoroalkyl and Polyfluoroalkyl Substances in Water by Direct Injection LC-MS/MS**; Jingcun Wu[1]; Erasmus Cudjoe[1]; SHENG-SUAN (victor) Cai[2]; Tyrally Ordinario[1]; Jacob Jalali[2]; Li-Zhong Yang[3]; <u>Feng Qin</u>[1]; [1]*PerkinElmer Inc., Woodbridge, ON;* [2]*Perkin Elmer, Waltham, MA;* [3]*PerkinElmer Management Co.,, Shanghai, China*

TP 153   **PFAS – Targeted & Non-Targeted High-Resolution Accurate Mass Analysis: Quick & Almost Effortlesss**; <u>Joseph Mick</u>[1]; Andrea Moberly[1]; [1]*Heritage Research Group, Indianapolis, IN*

TP 154   **Statistical approach for the analysis of contaminants of emerging concern (CECs) in complex water samples during treatment processes**; <u>Zsuzsanna Varga</u>[1]; Edith Nicol[1]; Yao Xu[1, 2]; Marc Lavielle[1, 2]; Stéphane Bouchonnet[1]; [1]*Ecole Polytechnique, Palaiseau, France;* [2]*National Institute for Research in Computer Science and Automation (Inria), Saclay, France*

TP 155   **Origins of contamination of the Earth atmosphere with pyridines**; <u>Albert T Lebedev</u>[1]; Olga Polyakova[1]; Alexander Kozhevnikov[2]; Nikolai Uljanovskii[2]; Dmitry Kosyakov[2]; Sergey Pokryshkin[2]; Tomas Latkin[2]; Vera Berzhonskis[3]; [1]*Moscow State University, Moscow, Russian Federation;* [2]*Northern (Arctic) Federal University, Arkhangelsk, Russia;* [3]) *Northern (Arctic) Federal University, Arkhangelsk, Russia*

TP 156   **Development and application of portable GC-MS for rapid determination of trace combustion supporting materials in fire scene**; <u>Jiancheng Yu</u>[1, 2]; Keqi Tang[1]; [1]*Ningbo University, Ningbo, China;* [2]*Ningbo Banff Biotech Inc., Ningbo, China*

TP 157   **Rapid Extraction of PCBs, Chlorinated Pesticides and PAHs in Sediment Sample and Analysis by GC-MS/MS Using Classical- and Pseudo-MRM Modes**; <u>Raj Mahat</u>[1]; Andy Ommen[1]; [1]*MilliporeSigma, Laramie, WY*

TP 158   **Proteomics analysis of whloe-body responses in medaka (Orysias latipes) esxposed to benzalkonium chloride**; <u>Young Sang Kwon</u>[1]; Jong Cheol Shon[1]; Yeong-Jin Kim[1]; Sung-Gil Choi[1]; Jong-Hwan Kim[1]; Jong-Su Seo[1]; [1]*Korea Institute of Toxicology, Munsan-eup, Jinju, South Korea*

TP 159   **Unveiling unknown toxicity-driven disinfection by-products in drinking waters: A combination of effect-directed analysis and 21 T FT-ICR**; <u>Huiyu Dong</u>[1, 2]; Amy A. Cuthbertson[1, 3]; Susan D. Richardson[1]; [1]*University of South Carolina, Columbia, SC;* [2]*Chinese Academy of Sciences, Beijing, China;* [3]*University of California, Berkeley, Berkeley, CA*

TP 160   **Testing the Removal of Microcystins from Water Using a Column Packed with Rice Husk**; <u>Sharmila I Thenuwara</u>[1]; David Baliu-Rodriguez[1]; Jon R Kirchhoff[1]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH*

TP 161   **The first Global surveillance study of organic micro-pollutants in riverine environments and drinking water using HRAM LCMSMS and Compound Discoverer**; Neville Llewellyn[1]; John Wilkinson[2]; Brett Sallach[3]; Ramón González-Méndez[4]; Olaf Scheibner[5]; Christina Jacob[6]; Martin Jech[5]; [1]*ThermoFisherScientific, Hemel Hempstead, United Kingdom; [2]York University, York, United Kingdom; [3]York University, York, United Kingdom; [4]Coventry University, Coventry, United Kingdom; [5]Thermo Fisher Scientific, Dreieich, Germany; [6]Thermo Fisher Scientific, San Jose, California*

TP 162   **Simultaneous determination of phthalate metabolites in dried blood spot (DBS) and saliva using liquid chromatography-tandem mass spectrometry (LC-MS/MS)**; Jiyoun Lee; *Department of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea*

TP 163   **Regional Level Variability of Poly- and Perfluoroalkyl Substances in Precipitation**; Kyndal Anne Pike[1]; Jennifer A. Faust[1]; Paul L. Edmiston[1]; Jillian Morrison[1]; [1]*The College of Wooster, Wooster, OH*

TP 164   **Demonstrating Improvements in PFAS Sensitivity Using a Microflow LC Approach for the EPA 537 Panel**; Katherine Hyland[1]; Karl Oetjen[2]; Simon Roberts[3]; Diana Tran[3]; [1]*SCIEX, Redwood City, CA; [2]SCIEX, Redwood Shores, California 1201; [3]SCIEX, Redwood Shores, CA*

TP 165   **Evaluating Removal Efficiency of CECs in Decentralized Wastewater Treatment Technologies using GCxGC/TOF-MS**; Jade L Johnson[1]; Eunha Hoh[1]; Natalie Mladenov[2]; Nathan G Dodder[1]; William H Richardot[1]; Lauren Steinberg[2]; [1]*School of Public Health, San Diego State University, San Diego, CA; [2]Department of Civil, Construction, and Environmental Engineering, San Diego State University, San Diego, CA*

TP 166   **Analysis of cotinine and trans-3-hydroxycotinine in dried urine spots from infants by liquid chromatography-tandem mass spectrometry**; Sumin Seo; *84, Heukseok-ro, Dongjak-gu, Seoul, Republic of Korea, seoul, South Korea*

TP 167   **FT-ICR MS Reveals the Structural Dependence for Generation of Recalcitrant Petroleum Contaminants**; Martha Liliana Chacon-Patino[1, 2]; Sydney F. Niles[1, 2]; Taylor J. Glattke[1, 2]; Amy Mckenna[1, 2]; Donald F. Smith[1, 2]; Alan G. Marshall[1, 2]; Christopher L. Hendrickson[1, 2]; Ryan P. Rodgers[1, 2]; [1]*Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*

TP 168   **Real time analysis of toluene degradation in a dielectric barrier discharge plasma**; Michel Heninger[1]; Essyllt Louarn[1]; Helene Mestdagh[1]; Joel Lemaire[1]; Stephane Pasquiers[2]; Nicole Blin-Simiand[2]; [1]*ICP, CNRS, Université Paris Saclay, Orsay, France; [2]LPGP, CNRS, Université Paris Saclay, Orsay, France, Orsay, France*

TP 169   **Formation of Disinfection By-Products during the Chlorination of Freshwater Algae Lyngbya wollei, Microcystis aeruginosa, and Algal Toxin Saxitoxin**; Md. Tareq Aziz[1]; Danielle C. C. Westerman[1]; Amy A. Cuthbertson[2]; Sam Putnam[1]; John L. Ferry[1]; Susan D. Richardson[1]; Leanne Powers[3]; Michael Gonsior[3]; [1]*University of South Carolina, Columbia, SC; [2]University of California, Berkeley, Berkeley, CA; [3]University of Maryland, Cambridge, MD*

TP 170   **Naphthenic Acids in Simulated Oil Spill and Constructed Wetland Plant Samples Using Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS)**; Joseph Monaghan[1]; Lindsay Hounjet; Stanislav R. Stoyanov[2]; John V. Headley[3]; Kerry M. Peru[3]; Christopher G. Gill[1]; Erik T. Krogh[1]; [1]*Applied Environmental Research Laboratories, Chemistry, Vancouver Island University, Nanaimo, BC; [2]Natural Resources Canada, Devon, AB; [3]Environment and Climate Change Canada, Saskatoon, SK*

TP 171   **An Alternative Ionization Technique For LC-MS/MS Analysis of Perfluoroalkyl Substances (PFAS) in Environmental Samples**; Kari Organtini[1]; Stuart Oehrle[1]; Kenneth Rosnack[1]; [1]*Waters Corporation, Milford, Massachusetts*

EPIGENETIC MODIFICATIONS
TP 172-178

TP 172   **Detection and/or quantification of modified RNA by LC-MS/MS: a new tool of discovery of a cancer biomarker**; Aurore Attina[1]; Jerome Vialaret[1]; Amandine Amalric[2]; Hélène Guillorit[2]; Amandine Bastide[2]; Sébastien Relier[2]; Eric Rivals[3]; Emmanuelle Samalin[4]; Evelyne Crapez[4]; Sylvain Lehmann[1]; Alexandre David[2]; Christophe Hirtz[1]; [1]*IRMB, Univ Montpellier, INSERM, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France; [2]Institute for Functional Genomics, Montpellier, France; [3]Laboratory of Computer Science, Robotics and Microelectronics of Montpellier, Montpellier, France; [4]Cancer Institute of Montpellier, Montpellier, France*

TP 173   **Enhancing bottom-up and middle-down proteomics data analysis for the identification of combinatorial histone post-translational modifications**; Seungjin Na[1]; Eunok Paek[1]; [1]*Hanyang University, Seoul, South Korea*

TP 174   **Targeted Proteomic Analysis for Interrogating the Epitranscriptomic Regulations of Small GTPases**; Yen-Yu Yang[1]; Ming Huang[1]; Yinsheng Wang[1]; [1]*UC Riverside, Riverside, CA*

TP 175   **Global ubiquitination profiling of HIV-1-infected cells reveals mechanisms of host cellular chromatin remodeling**; Jeffrey Johnson[1]; Donna Li[2]; Oliver Fregoso[3]; Nevan Krogan[4, 5]; [1]*Icahn School of Medicine at Mount Sinai, New York, NY; [2]University of Wisconsin, Madison, WI; [3]University of California, Los Angeles, Los Angeles, CA; [4]University of California San Francisco, San Francisco, CA; [5]Gladstone Institutes, San Francisco, CA*

TP 176 **Systematic investigation of PRMT6 substrate recognition reveals broad specificity with a preference for basic and bulky residues**; <u>Joshua J Hamey</u>[1]; Sinja Rakow[2]; Caoline Bouchard[2]; Uta Maria Bauer[2]; Marc R Wilkins[1]; Gene Hart-Smith[1, 3]; [1]*School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia;* [2]*Institute for Molecular Biology and Tumor Research (IMT), Philipps-University Marburg, Marburg, Germany;* [3]*Department of Molecular Sciences, Macquarie University, Sydney, Australia*

TP 177 **Investigating the role of phosphorylation in the regulation of the S. cerevisiae lysine demethylase Rph1 using LC-MS/MS**; <u>Mandy W. M. Wong</u>[1]; Ryan J. Separovich[1]; Marc R Wilkins[1]; [1]*Systems Biology Initiative UNSW, Sydney, Australia*

TP 178 **The role of upstream phosphorylation in the regulation of histone methylation**; <u>Ryan J. Separovich</u>[1]; Joshua J Hamey[1]; Marc R Wilkins[1]; [1]*School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia*

FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS II
TP 179-192

TP 179 **Development and Evaluation of a Multifaceted LC-HRMS/MS Method for the Screening of Adulterants in Dietary Supplements**; <u>Christopher R. Beekman</u>[1]; Rahul Pawar[1]; [1]*U.S. Food and Drug Administration, College Park, MD*

TP 180 **Atmospheric Solid Analysis Probe mass spectrometry for food compliance screening: oregano authenticity case study**; <u>Tito Damiani</u>[1]; Nicola Dreolin[2]; Sara Stead[2]; Chiara Dall'asta[1]; [1]*University of Parma, Parma, Italy;* [2]*Waters Corporation, Wilmslow, United Kingdom*

TP 181 **Potential of trapped-ion-mobility UHPLC-QTOF in food authenticity studies: characterization of co-eluting secoiridoids isomers found in Greek extra virgin olive oil**; Sofia K. Drakopoulou[1]; Dimitrios E Damalas[1]; Nikolaos S. Thomaidis[1]; <u>Carsten Baessmann</u>[2]; [1]*National and Kapodistrian University of Athens, Athens, Greece;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

TP 182 **Evaluation of a compact LC-TOF platform as an accessible screening technique for unexpected contaminants in foods, and food supplements**; Sara Stead[1]; Emmanuelle Claude[1]; Christopher Henry[1]; <u>Steve Preece</u>[1]; Kenneth Rosnack[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Waters Corporation, Darlington, PA*

TP 183 **Investigations into Small Molecule Pesticide Protomers and Conformers Using Linear and Cyclic Ion Mobility Separators**; Mike_mccullagh@waters.com Mccullagh[1]; Martin Palmer[1]; Jakub Ujma[1]; <u>Emma Marsden-Edwards</u>[1]; Séverine Goscinny[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Sciensano, Brussels, Belgium*

TP 184 **Real-time monitoring of frying fumes composition using proton transfer reaction mass spectrometry**; <u>Tomasz Majchrzak</u>[1]; Wojciech Wojnowski[1]; Agnieszka Głowacz-Różyńska[2]; Andrzej Wasik[1]; [1]*Gdansk University of Technology, Department of Analytical Chemistry, Gdansk, Poland;* [2]*Gdansk University of Technology, Department of Colloid and Lipid Science, Gdansk, Poland*

TP 185 **A cross-platform (PRM/SRM) targeted method for quantitation of peanut residues**; <u>Justin T Marsh</u>[1]; Charles Yang[2]; Philip E Johnson[3]; [1]*University of Nebraska Lincoln, Lincoln, NE;* [2]*ThermoFisher Scientific, San Jose, CA;* [3]*University of Nebraska-Lincoln, Lincoln, NE*

TP 186 **An MRM-based Method for Quantitative Analysis of Functional Carotenoids in Biological and Food Samples**; <u>Zhe Sun</u>[1]; Jie Xing[1]; Hui Zhang[1]; Nicole Jia Min Chen[2]; Zhaoqi Zhan[1]; [1]*Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore;* [2]*National University of Singapore, Singapore, Singapore*

TP 188 **LC-QTOF-MS identification of rabbit-specific peptides for meat species control in meat products**; Anna Stachniuk[1]; Agata Sumara[1]; Magdalena Montowska[2]; <u>Emilia Fornal</u>[1]; [1]*Medical University of Lublin, Lublin, Poland;* [2]*Poznan University of Life Sciences, Poznan, Poland*

TP 189 **Selection of peptide targets for species-independent quantitation of fish allergens**; Justin T Marsh[1]; Charles Yang[2]; <u>Philip E Johnson</u>[3]; [1]*University of Nebraska Lincoln, Lincoln, NE;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*University of Nebraska-Lincoln, Lincoln, NE*

TP 190 **Beer processomics: Untargeted profiling of volatile and nonvolatile compounds throughout the production of a single hop, single malt (SMaSH) beer**; <u>Lynn E. Marsh</u>[1]; Adrianna R. Losquadro[1]; Ashleigh E. Outhous[1]; Samuel A. Morton[1]; Steven Harper[1]; Christine A. Hughey[1]; [1]*James Madison University, Harrisonburg, VA*

TP 191 **Rapid UHPLC Identification of Anthocyanins from Different Varieties of Berries using High Resolution-QTOF-Mass spectrometry**; <u>Jashbir Singh</u>[1]; Jayashan Adhikari[2]; G. K. Jayaprakasha[2]; Bhimanagouda S. Patil[2]; [1]*Texas A & M University, College Station, TX;* [2]*Texas A&M University, College Station, TX*

TP 192 **Aquaculture Proteomics for the Evaluation of Antibacterial Feed on Paralichthys Olivaceus**; <u>Jihoon Shin</u>[1]; Min-gyu Youn[1]; Miseon Jeong[1]; Junghoon Kang[1]; Youngjin Kim[1]; Wonryeon Cho[1]; [1]*Wonkwang University, Iksan, South Korea*

GLYCOPROTEINS II
TP 193-209

TP 193 **Spot the Differences: Assessing site-specific glycosylation similarity between influenza A virus variants with statistical certainty**; Deborah Chang[1]; William E Hackett[2]; Joshua A Klein[2]; Joseph Zaia[1, 2]; [1]*Boston University School of Medicine, Boston, MA;* [2]*Bioinformatics Program, Boston University, Boston, MA*

TP 194 **Characterization of High Mannose and Phosphorylated High Mannose Glycosylation Sites in Hybrid β-Hexosaminidase (HexM)**; Taylor Battellino[1]; Tyler Tran[1]; Duc Minh Nguyen[1]; Graeme Benzie[1]; Oleg Krokhin[1]; Brian Mark[1]; Helene Perreault[1]; [1]*University of Manitoba, Winnipeg, MB*

TP 195 **Enrichment Assisted Identification of Glycosylated Neuropeptides in Crustaceans**; Ashley Phetsanthad[1]; Lingjun Li[1, 2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

TP 196 **Glycosylation Patterns in Neoplastic Biomarker Alpha Fetoprotein in Pathologic Human Serum Samples**; Mark M Kushnir[1]; Yifei K Yang[1, 2]; [1]*ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT;* [2]*University of Utah, Salt Lake City, UT*

TP 197 **Optimization of glycoproteome analysis workflow using Chinese Hamster Ovary Cells**; Hsiang-En Hsu[1]; Raghothama Chaerkady[1]; Matthew Glover[1]; Gargi Roy[1]; Sonja Hess[1]; [1]*R&D, AstraZeneca, Gaithersburg, MD*

TP 198 **Evaluation of O-glycosylation via O-glycan specific Proteolysis, LC-MS and Rapid Data Processing**; Charles Nwosu[1]; Lei Wang[2]; Yan Wang[2]; Chris Barton[2]; [1]*Takeda Pharmaceuticals International Co, Cambridge, MA;* [2]*Takeda Pharmaceuticals International Co., Cambridge, MA*

TP 199 **Systematic examination of protein/glycopeptide extraction methods and MS/MS fragmentation techniques for monitoring human milk glycoproteins survival across preterm infant digestion**; Bum Jin Kim[1]; Marshall Bern[2]; David C. Dallas[1]; [1]*Oregon State University, Corvallis, OR;* [2]*Protein Metrics Inc., Cupertino, CA*

TP 200 **Enrichment-free O-glycoproteome based on Trapped Ion Mobility Q-TOF**; Xue Sun[1]; Wenmin Tian[1]; Jianhui Cheng[2]; Ning Chen[3]; Yang Chen[1]; Catherine C L Wong[1]; [1]*Center for Precision Medicine Multi-Omics Research, Peking University, Beijing, China;* [2]*Department of Chemistry, University of British Columbia, Vancouver, BC;* [3]*Bruker Daltonics, Beijing, China*

TP 201 **Quantitative O glycosylation characterization in fetuin by hot electron capture dissociation, detection of more than fifty O glycopeptides**; Takashi Baba[1]; Suya Liu[1]; Pavel Ryumin[1]; [1]*SCIEX, Concord, ON*

TP 202 **Improving UPLC/MS N-glycosylation analysis of disulfide-rich fusion proteins through optimization of sample preparation conditions**; Ximo Zhang[1]; Mauro Sassi[2]; Erika Birolo[2]; Paolo Felici[2]; Nunzio Sepe[2]; Antonio Datola[2]; Robert Birdsall[1]; Ying-Qing Yu[1]; [1]*Waters Corps, Milford, MA;* [2]*Merck Serono S.p.A., Rome, Italy*

TP 203 **Analysis of Multiply-Fucosylated Epidermal Growth Factor Receptor (EGFR) Glycopeptides in Oral Squamous Cell Carcinoma via HCD and EThcD**; Kevin Brown Chandler[1]; Vanessa L Stahl[1]; Bach-Cuc Nguyen[2]; Maria A Kukuruzinska[2]; Catherine E. Costello[1]; [1]*Center for Biomedical Mass Spectrometry, Department of Biochemistry, Boston University School of Medicine, Boston, Massachusetts;* [2]*Department of Translational Dental Medicine, Boston University School of Dental Medicine, Boston, Massachusetts*

TP 204 **Large Scale Analysis of Sialic Linkage Isomers from Intact Glycopeptides Revels Structural Diversity**; Jonathan C. Trinidad[1]; Kathleen T. Grassmyer[1]; Xuyao Zeng[1]; David E. Clemmer[1]; [1]*Indiana University, Bloomington, IN*

TP 205 **Optimizing the duration of hydrazine hydrate chemical deglycosylation for MS analysis of mucin-type O-linked glycans**; Bryan E Hettick[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

TP 206 **RAMZIS: a bioinformatic tool for rigorous assessment glycoprotein similarities from LC-tandem mass spectrometric data**; William E Hackett[1]; Deborah Chang[2]; Luis Carvalho[3, 4]; Joseph Zaia[2, 4]; [1]*Boston University, Boston, MA;* [2]*Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA;* [3]*Department of Mathematics, Boston University, Boston, MA;* [4]*Bioinformatics Program, Boston University, Boston, MA*

TP 207 **Two-Dimensional Electron Capture Dissociation Fourier Transform Ion Cyclotron Resonance Mass Spectrometric Analysis of N-Linked Glycopeptides**; Richard J Bell[1]; Eric D Dodds[1]; [1]*University of Nebraska-Lincoln, Lincoln, NE*

TP 208 **Comprehensive N- and O-glycosylation characterization of multiple CHO host cell lines using HILIC-GIG method**; Qiong Wang[1]; Shuang Yang[2]; Tiexin Wang[1]; Michael J. Betenbaugh[1]; John Cipollo[2]; Yuan Tian[2]; [1]*JHU Chemical Engineering Department, Baltimore;* [2]*FDA Laboratory for Bacterial Polysaccharides, Silver Spring, Maryland*

TP 209 **An automated MS data workflow enabling targeted, site-specific glycosylation monitoring in continuous biopharmaceutical manufacturing**; Bertaccini Diego; *Merck KGaA, Corsier-sur-Vevey, Switzerland*

IMAGING MS: DISEASE MARKERS
TP 210-227

TP 210 **Dissecting Protein Signature of Soy Diet in Fragile X Mouse Model Using MALDI-Imaging Mass Spectrometry Combined with Shotgun Proteomics**; Min Ma[1]; Qinying Yu[1]; Pamela R. Westmark[2]; Cara J. Westmark[2]; Lingjun Li[1, 3]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Neurology, University of Wisconsin-Madison, Madison, WI;* [3]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 211 **MALDI Mass Spectrometry Imaging revealed Neutrophil Defensins as new Predictive Biomarkers for Immunotherapy Response in NSCLC Patients**; Eline Berghmans[1, 2]; Geert Baggerman[1, 2]; [1]*Centre for Proteomics, Antwerpen, Belgium;* [2]*Unit Health (VITO), Mol, Belgium*

TP 212 **MALDI IMS and Comparative Pathology: Defining Molecular Constituents of Staphylococcal Tissue Abscess Formation and Maturation**; William J Perry[1, 2, 3]; Andy Weiss[3, 4]; Kelli L Boyd[4]; Nathan Heath Patterson[5, 6]; Jeffrey M Spraggins[2, 5, 6]; Eric P Skaar[3, 4]; Richard M Caprioli[2, 5, 6, 7, 8]; [1]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [2]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [3]*Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University, Nashville`, TN;* [4]*Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN;* [5]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205;* [6]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [7]*Department of Pharmacology, Vanderbilt University, Nashville, TN;* [8]*Department of Medicine, Vanderbilt University, Nashville, TN*

TP 213 **Comparison of plasma and tissue lipidome for the investigation of molecular signatures of breast cancer**; Alex A. R. Silva[1]; Marcella Cardoso[2]; John Q Lin[3]; Charlotte Hueblauer[4]; Geisilene R. P. Silva[2]; Marcos N. Eberlin[5]; Livia S. Eberlin[3]; Sophie F. M. Derchain[2]; Andreia M. Porcari[1]; [1]*Laboratory of Multidisciplinary Research, São Francisco University, Bragança Paulista, Brazil;* [2]*Department of Gynecological and Breast Oncology, Women's Hospital (CAISM), Faculty of Medical Sciences, State University of Campinas (UNICAMP), Campinas, Brazil;* [3]*Department of Chemistry, The University of Texas at Austin, Austin, texas;* [4]*Medical University of Graz, Graz, Austria;* [5]*Mackenzie Presbyterian University, School of Engineering, São Paulo, Brazil*

TP 214 **Molecular characterization of NAFLD-related liver cancer in pig using MALDI imaging mass spectrometry and shotgun proteomics**; Kohta Iguchi[1, 2]; Mayuka Kosugi[3]; Naohiko Nakamura[2]; Takashi Nirasawa[4]; Ryo Kajita[4]; Etsuro Hatano[2]; Shugo Ueda[1]; Hiroaki Terajima[1]; Shinji Uemoto[2]; Masaya Ikegawa[3]; [1]*Kitano Hospital, The Tazuke Kofukai Medical Research Institute, Osaka, Japan;* [2]*Department of Surgery, Graduate School of Medicine, Kyoto University, Kyoto, Japan;* [3]*Department of Life and Medical Systems, Faculty of Life and Medical Sciences, Doshisha University, Kyotanabe, Japan;* [4]*Bruker Japan, Yokohama, Japan*

TP 215 **Dissecting Rostral Migratory Stream (RMS) through MALDI-Imaging Mass Spectrometry on murine olfactory deprivation model**; Daiki Kameyama[1]; Takashi Nirasawa[2]; Ryo Kajita[2]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; [1]*Faculty of Life and Medical Science, Department of Life and Medical Systems, Doshisha University, Kyotanabe City, Japan;* [2]*Bruker Japan K.K., Yokohama, Japan*

TP 216 **Unraveling pathogenesis of dilated cardiomyopathy (DCM) on J2N-k Hamster model using MALDI-Imaging Mass Spectrometry in combination with shotgun proteomics**; Inori Shintani[1]; Takashi Tsuji[2]; Mizuki Ishida[1]; Takashi Nirasawa[3]; Ryo Kajita[3]; Hatsue Ishibashi-Ueda[4]; Hidetoshi Masumoto[2]; Kenji Minatoya[2]; Masaya Ikegawa[1]; [1]*Doshisha University, Kyotanabe, Japan;* [2]*Kyoto University, Kyoto, Japan;* [3]*Bruker Japan K.K., Yokohama, Japan;* [4]*National Cerebral and Cardiovascular Center, Suita, Japan*

TP 217 **Unraveling Tissue Complexity in Samples of Human Inflammatory Bowel Disease Using Imaging Mass Spectrometry**; Simona Salivo[1]; Lucia Martín-Saiz[2]; Albert Maimó-Barceló[3]; Javier Martín[2]; Juan J. Gutiérrez[2]; Joan Bestard-Escalas[3]; Daniel H. López[3]; Sam Khorrami[3, 4]; Marcelo García[3, 4]; Tom K. Abban[1]; Matthew E. Openshaw[1]; Gwendolyn Barceló-Coblijn[3]; José A. Fernández[2]; [1]*Shimadzu, Manchester, UK, Manchester, United Kingdom;* [2]*Department of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena s/n, 48940, Spain;* [3]*Research Unit, Hospital Universitari Son Espases, Institut d'Investigació Sanitària Illes Balears(IdISBa), Palma, Spain;* [4]*Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain*

TP 218 **Mass Spectrometry Imaging to Differentiate between Pancreatic Adenocarcinoma and Cholangiocarcinoma**; Christine Bollwein[1]; Alice Ly[2]; Juliana Goncalves[1]; Sören-Oliver Deininger[2]; Wilko Weichert[1]; Kristina Schwamborn[1]; [1]*Institute of Pathology, Technical University Munich, Munich, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

TP 219 **High Resolution Imaging Mass Spectrometry of Human Donor Eyes with Retinal Pathology**; David M. G. Anderson[1]; Ankita Kotnala[1, 2]; Jarod A. Fincher[1]; Jeffrey D. Messinger[2]; Nathan Heath Patterson[1]; Jeffrey M Spraggins[1]; Christine A. Curcio[2]; Kevin L. Schey[1]; [1]*Vanderbilt University, Department of Biochemistry, Nashville, TN;* [2]*University of Alabama at Birmingham, Birmingham, AL*

TP 220   **Helicobacter pylori-induced Molecular Alterations in Gastric Tissue Visualized by Imaging Mass Spectrometry**; Michelle Reyzer[1]; Aung Soe Lin[1]; Jeff Shaw[1]; Ankita Kotnala[1]; Michael Tuck[1]; Jennifer Harvey[1]; Maria B. Piazuelo[1]; Kevin L. Schey[1]; Timothy Cover[1]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

TP 221   **Comparative Ultra-high Resolution Imaging MS Reveals Lipid and Fatty Acid Dyshomeostasis in a 3K a-Synuclein Parkinson's Disease-like Mouse Model**; Madison H. Mcminn[1, 2]; Silke Nuber[3]; Walid Abdelmoula[2]; Sylwia A. Stopka[2]; Dennis Selkoe[3]; Jeffrey N. Agar[1]; Nathalie Y. R. Agar[2, 4, 5]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Neurosurgery, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [3]Ann Romney Center for Neurologic Diseases, Department of Neurology, Brigham and Women's Hospital and Harvard Medical School, Boston, MA; [4]Department of Radiology, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [5]Department of Cancer Biology, Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA*

TP 222   **Mass Spectrometry imaging applied to study HIV-associated cardiovascular disease**; David O Ajasin[1]; Brendan Prideaux[1]; Eliseo Eugenin[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

TP 223   **Implementation of multimodal data to interpretation of results of rapid molecular profiling of brain tumors using MALDI-imaging**; Igor Popov[1, 2]; Evgeniy Zhvansky[1]; Daniil Ivanov[1]; Stanislav Pekov[1]; Anatoly Sorokin[1]; Vsevolod Shurkhay[1, 2]; Denis Zavorotnyuk[1]; Pavel Nikitin[2]; Alexander Potapov[2]; Eugene (evgeny) Nikolaev[3]; *[1]Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation; [2]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [3]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

TP 224   **Identification of Therapeutic Targets of Multiple Sclerosis through MALDI - Imaging Mass Spectrometry of Experimental Autoimmune Encephalomyelitis (EAE) mouse model**; Nami Tanaka[1]; Hiroki Yamashita[1]; Takashi Nirasawa[2]; Ryo Kajita[2]; Katsutoshi Taguchi[3]; Masaki Tanaka[3]; Takayuki Kondo[4]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyoto, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]Department of Anatomy and Neurobiology, Graduate School of Medical Science, Kyoto Prefectural University of Medicine, Kyoto, Japan; [4]Kansai Medical University Medical Center, Hirakata, Japan*

TP 225   **AP-SMALDI-MSI of Cryptosporidium parvum and Neospora caninum-infected cells and tissue**; Nils Anschütz[1]; Stefanie Gerbig[1]; Camilo Larrazabal[2]; Juan Velez[2]; Liliana Silva[2]; Carlos Hermosilla[2]; Anja Taubert[2]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany; [2]Institute of Parasitology, Justus Liebig University Giessen, Giessen, Germany*

TP 226   **A novel and promising proteomic-based MALDI-MSI thyroid nodule classifier as complementary diagnostic tool in cytopathology**; Isabella Piga[1]; Giulia Capitoli[1]; Francesca Clerici[1]; Allia Mahajneh[1]; Virginia Brambilla[2]; Vanna Denti[1]; Andrew Smith[1]; Stefania Galimberti[3]; Fulvio Magni[1]; Fabio Pagni[2]; *[1]University of Milano – Bicocca, Proteomics and Metabolomics platform, School of Medicine and Surgery, Vedano al Lambro, Italy; [2]University of Milano – Bicocca, School of Medicine and Surgery, Pathology Section, San Gerardo Hospital, ASST Monza, Italy; [3]University of Milano – Bicocca, Center of Biostatistics for Clinical Epidemiology, School of Medicine and Surgery, Vedano al Lambro, Italy*

TP 227   **Mapping the Spatial Distribution of Prostaglandin E2 (PGE2) in Tumor with DESI Ion Mobility-MS Imaging**; Bindesh Shrestha[1]; Anthony Midey[1]; Hernando Olivos[1]; Long Yuan[2]; Zhuyin Li[2]; Jia Peng[2]; Qihong Zhao[2]; Qin Ji[2]; *[1]Waters Corporation, Beverly, MA; [2]BMS Co., Princeton, NJ*

IMAGING MS: SMALL MOLECULES
TP 228-234

TP 228   **High Performance Thin-Layer Chromatography (HPTLC) of Ecdysteroids Present in Plant Extracts Coupled with in situ Analysis and Imaging DESI/IMS/MS**; Emmanuelle Claude[1]; Mark Towers[1]; Rene Lafont[2]; Ian D Wilson[3]; Robert Plumb[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Sorbonne Université, Campus Pierre et Marie Curie, IBPS-BIOSIPE, Paris, France; [3]Division of Systems Medicine, Department of Metabolism, Digestion and Reproduction, Imperial College London, South Kensington, United Kingdom; [4]Waters Corps, Milford, MA*

TP 229   **Spatial Distribution of Chemotherapeutics in Paper-based Cell Cultures via Infrared Matrix Assisted Laser Desorption Electrospray Ionization- Mass Spectrometry Imaging (IR-MALDESI-MSI)**; Tyler S Larson[1]; Elias P Rosen[1, 2]; Matthew R Lockett[1, 3]; Gary L Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]UNC Eshelman School of Pharmacy, Chapel Hill, NC; [3]Lineberger Comprehensive Cancer Center, University of North Carolina, Chapel Hill, NC*

TP 230   **Following chemotherapeutic drug distribution in three-dimensional cancer cell spheroids using MSI-TOF-SIMS and LESA-TIMS-MS**; Yarixa L Cintron-Diaz[1]; Arlet M. Acanda De La Rocha[1]; Anthony Castellanos[2]; Jeremy W. Chambers[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Florida International University, Miami, Florida*

TP 231   **Alterations in lipid profile of a depression model detected by MALDI-imaging mass spectrometry**; Jong Bok Seo[1]; Eui-Gil Jung[1]; Hee-Jung Kim[1]; Bong June Yoon[2]; Jinnyoung Choi[3]; *[1]Korea Basic Science Institute, Seoul, South Korea; [2]Korea University, Seoul, South Korea; [3]Bruker Korea, Seongnam, South Korea*

TP 233   **Rapid discrimination of Panax ginseng in different growing years using DESI-MS imaging coupled with chemometrics**; <u>Yuangui Yang</u>[1]; Yanchao Shi[2]; Yingbo Yang[3]; Kate Yu[1]; Ming Yuan[2]; Zhengtao Wang[4]; Li Yang[4]; [1]*Shanghai University of Traditional Chinese Medicine, Shanghai, China;* [2]*Waters Corporation Shanghai Science & Technology Co Ltd, shanghai, China;* [3]*Kanion Pharmaceutical Co., Ltd, Jiangsu, Lianyungang, China;* [4]*Shanghai University of Traditional Chinese Medicine, shanghai, China*

TP 234   **Mass Spectrometry Imaging in Cesium Mapping for Thermochemical Ablation: Correlation with Dual-Energy Computed Tomography**; <u>Emily A. Thompson</u>[1]; Dodge L. Baluya[1, 2]; A. Colleen Crouch[1]; Megan C. Jacobsen[1]; Rick R. Layman[1]; Elizabeth M. Whitley[1]; Erik N.K. Cressman[1]; [1]*MD Anderson Cancer Center, Houston, TX;* [2]*Washington State University, Pullman, WA*

INFORMATICS: WORKFLOW AND DATA MANAGEMENT
TP 235-248

TP 235   **New data flow model for rapid automated processing of large volumes of LC/UV/MS data**; <u>Richard Lee</u>[1]; Andrey Paramonov[1]; Vladislav Solomatin[1]; Eugene Volopianov[1]; [1]*ACD/Labs, Toronto, ON*

TP 236   **high-throughput labeled LC-MS/MS data normalization and automated reporting**; <u>Joris Van Houtven</u>[1, 2, 3]; Evelyne Maes[4]; Kris Laukens[5]; Geert Baggerman[2, 3]; Jef Hooyberghs[2]; Dirk Valkenborg[1, 2, 3]; [1]*Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Data Science Institute, Hasselt University, Hasselt, Belgium;* [2]*Flemish Institute for Technological Research (VITO), Mol, Belgium;* [3]*Centre for Proteomics, Antwerpen, Belgium;* [4]*AgResearch, Christchurch, New Zealand;* [5]*Biomina, Antwerpen, Belgium*

TP 237   **A new version of the PRIDE database including a new interactive website and Restful API**; <u>Suresh C Hewapathirana</u>[1]; Jingwen Bai[1]; Chakradhar Bandla[1]; David García-Seisdedos[1]; Selvakumar Kamatchinathan[1]; Deepti J. Kundu[1]; Juan Antonio Vizcaino[1]; [1]*European Bioinformatics Institute, Cambridge, United Kingdom*

TP 238   **New Functionalities in proteoQ: Facile Integration of Data Normalization and Informatic Analysis for Quantitative Proteomic Workflows Using Tandem Mass Tags**; <u>Qiang Zhang</u>[1]; R Reid Townsend[1]; [1]*Washington University School of Medicine, St. Louis, MO*

TP 239   **Towards a Computational Workflow for the Analysis of DOM Fragmentation Data**; <u>Muhammad Usman Tariq</u>[1]; Dennys Leyva[1]; Francesco Fernandez-Lima[1]; Fahad Saeed[1]; [1]*Florida International University, Miami, FL*

TP 240   **LC-MS/MS system suitability evaluation with automated data processing for protein analysis in a regulated environment**; <u>Wencheng Ge</u>[1]; Bhavin Patel[1]; [1]*Thermo Fisher Scientific, Rockford, IL*

TP 241   **Updates on Philosopher: a complete toolkit for both conventional and open search-based shotgun proteomics data analysis**; <u>Felipe Da Veiga Leprevost</u>[1]; Sarah E. Haynes[1]; Fengchao Yu[1]; Avinash K. Shanmugam[1]; Dattatreya Mellacheruvu[1]; Hui-Yin Chang[1]; Dmitry M. Avtonomov[1]; Andy Kong[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

TP 242   **A data analysis pipeline for quality control and differential expression analysis of quantitative proteomics**; <u>Frank Koopmans</u>[1]; Miguel A Gonzalez-Lozano[1]; August B Smit[1]; Ka Wan Li[1]; [1]*VU university, Amsterdam, Netherlands*

TP 243   **MassIVE: bridging the gap between data and discovery through large-scale reanalysis**; <u>Jeremy Carver</u>[1]; Julie Wertz[1]; Benjamin Pullman[1]; Nuno Bandeira[1]; [1]*UCSD, La Jolla, CA*

TP 244   **SimpliFi: a GPU-driven data-to-meaning analytics engine to bring omics understanding to all**; <u>Jim Palmeri</u>[1]; Darryl J. Pappin[1, 2]; John Wilson[1]; [1]*ProtiFi, LLC, Farmingdale, New York;* [2]*Cold Spring Harbor Laboratory, COLD SPRING HARBOR, New York*

TP 245   **Production and Generation of Proteogenomics Databases using PyPGATK**; <u>Husen M. Umer</u>[1]; Yafeng Zhu[2]; Enrique Audain[3]; Janne Lehtiö[1]; Rui Branca[1]; Yasset Perez-Riverol[4]; [1]*Department of Oncology-Pathology, Science for Life Laboratory, Karolinska Institutet, Stockholm, Sweden;* [2]*Department of Genetics, Harvard Medical School, Boston, MA 02115;* [3]*Department of Congenital Heart Disease and Pediatric Cardiology, Universitätsklinikum Schleswig–Holstein Kiel, Kiel, Germany;* [4]*European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus, Hinxton, Cambridge, United Kingdom*

TP 246   **DIA-expert Cloud: A fast, efficient cloud-based framework in Amazon for DIA data analytics**; <u>Chen Hao</u>[1]; Xiaoxu Zhou[2]; Meng Luo[2]; Tiansheng Zhu[2]; Tiannan Guo[2]; Lu Li[2]; [1]*Westlake University, hangzhou, China;* [2]*Westlake University, Hangzhou, China*

TP 247   **"TimsPy": access timsTOF Pro data easily from Python**; <u>Mateusz Krzysztof Lacki</u>[1]; Sven Brehmer[2]; Ute Distler[1]; Stefan Tenzer[1]; [1]*University Medical Center, Johannes Gutenberg University, Mainz, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

TP 248   **Scalability Redefined: A new workflow in Spectronaut to analyze 10'000+ raw files on a desktop workstation**; <u>Oliver M. Bernhardt</u>[1]; Jakob Vowinckel[1]; Tejas Gandhi[1]; Lukas Reiter[1]; [1]*Biognosys AG, Schlieren, Switzerland*

INSTRUMENTATION: NEW CONCEPTS
TP 249-258

TP 249   **Flexible Ion Guides: The Missing Link in Ambient Ionization Mass Spectrometry**; <u>Mazdak Taghioskoui</u>[1]; Charles Wang[2]; [1]*Trace Matters Scientific LLC, Somerville, MA;* [2]*Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts*

TP 250   **Mass Spectrometer Observing Lunar Operations (MSolo)**; <u>Roberto Aguilar</u>[1]; Janine E. Captain[1]; Jacqueline W. Quinn[1]; Julie E. Kleinhenz[2]; Kenneth Wright[3]; Jorge Andres Diaz[3]; James D. Fox[3]; Jaime Winfield[3]; Peter Santariello[3]; Kris Zacny[4]; Zachary Mank[4]; Gale Paulsen[4]; [1]*National Aeronautics and Space Administration, Kennedy Space Center, FL;* [2]*National Aeronautics and Space Administration, Johnson Space Center, TX;* [3]*INFICON, Syracuse, NY;* [4]*Honeybee Robotics, Altadena, CA*

TP 251   **Hyperthermal Ion Beam Deposition Using a Rotating Wall Mass Analyzer**; Pei Su[1]; <u>Michael Forrester Espenship</u>[1]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN*

TP 252   **An optimized PTR3-TOFMS instrument for high-sensitivity and high-resolution analysis in atmospheric research and environmental chemistry**; <u>Tobias Reinecke</u>[1]; Alfons Jordan[1]; Markus Leiminger[1]; Stefan Feil[1]; Christian Lindinger[1]; Lukas Märk[1]; Philipp Sulzer[1]; [1]*IONICON Analytik GmbH., Innsbruck, Austria*

TP 253   **Ion Manipulation Effects Inside a Digitally Driven Quadrupole**; <u>Margaret E. Reece</u>[1]; Adam P. Huntley[1]; Conner F. Bailey[1]; Sumeet Chakravorty[1]; Peter T.A. Reilly[1]; [1]*Washington State University, Pullman, WA*

TP 254   **Computational Evaluation of Sine and Rectangular Wave Mass Filter Acceptance and Transmittance Influenced by Developing Fields**; <u>Adam P Huntley</u>[1]; Peter T. A. Reilly[1]; [1]*Washington State University, Pullman, WA*

TP 255   **A novel ion optical device to improve duty cycle of a Q-TOF mass spectrometer**; <u>Xiaoqiang Zhang</u>[1]; Wenjian Sun[1]; Lin Liu[1]; Liping Huang[1]; [1]*Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China*

TP 256   **Construction of a miniature digital rectilinear ion trap (DRIT) mass spectrometer**; <u>Han Bin Oh</u>[1]; Jae-ung Lee[1]; Igor Filippov[2]; [1]*Sogang Univ. Dept. of Chemistry, Seoul, South Korea;* [2]*Auckland Univ. Dept. of Physics, Auckland, New Zealand*

TP 258   **Fundamental Principles and Performance for a Low Vacuum Mass Spectrometer**; <u>Yiming Lin</u>[1]; Wenjian Sun[1]; Qiao Jin[1]; Hongbing Cheng[1]; [1]*Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING I
TP 260-279

TP 260   **Nanosecond pulsed dielectric barrier discharge ionization mass spectrometry**; <u>Ezaz Ahmed</u>[1]; Dan Xiao[2]; Morphy C. Dumlao[1, 3, 4, 5]; Christopher C. Steel[3, 4]; Leigh M. Schmidtke[3, 4, 5]; John Fletcher[2]; William A. Donald[1]; [1]*School of Chemistry, University of New South Wales, Sydney, Australia;* [2]*School of Electrical Engineering and Telecommunications, University of New South Wales, Sydney, Australia;* [3]*School of Agricultural and Wine Sciences, Charles Sturt University, Wagga Wagga, Australia;* [4]*National Wine and Grape Industry Centre, Charles Sturt University, Wagga Wagga, Australia;* [5]*Australian Research Council Training Centre for Innovative Wine Production, University of Adelaide, Glen Osmond, Australia*

TP 261   **A soft ionization source for generating, storing, and ejecting positive and negative ions**; <u>Qinghao Wu</u>[1]; Xiaofeng Zhao[1]; [1]*IonX Tech, LLC, Richland, WA*

TP 262   **Investigating Hypervelocity Surface-induced Racemization Reactions Prior to Ionization & Mass Analysis of Gas Phase Amino Acids During Flyby Sampling**; <u>Abraham L De La Cruz Hernandez</u>[1]; Daniel E. Austin[1]; Eric T. Sevy[1]; [1]*Brigham Young University, Provo, UT*

TP 263   **A Proton-Transfer-Reaction – Mass Spectrometry (PTR-MS) Setup with Real-Time Response for Low-Volatile Compounds**; <u>Alfons Jordan</u>[1]; Felix Piel[1, 2]; Markus Müller[1]; Jenny Skytte af Sätra[2]; Klaus Winkler[1]; Tobias Reinecke[1]; Christian Lindinger[1]; Armin Wisthaler[2]; Lukas Märk[1]; Philipp Sulzer[1]; [1]*IONICON Analytik GmbH., Innsbruck, Austria;* [2]*Department of Chemistry, University of Oslo, Oslo, Norway*

TP 264   **Gas Chromatography-Atmospheric Flow Tube-Mass Spectrometry (GC-AFT-MS) Analysis of Post-Detonation Explosive Residues**; <u>Kelsey A. Morrison</u>[1]; Elizabeth H. Denis[1]; Robert G. Ewing[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

TP 265   **Enhanced Ionization and Facile Selection of Ions at Atmospheric-pressure by Perturbation-induced Pulsing of nano-ESI Coupled to a Single Ion Gate**; <u>William P. McMahon</u>[1]; Kaveh Jorabchi[1]; [1]*Georgetown University, Washington, DC*

TP 266   **Experimental Investigation of Charged Nanodroplets in MS Transfer Stages originating from ESI plumes**; <u>Florian Stappert</u>[1]; Clara Markert[1]; Marco Thinius[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany*

TP 267   **An Integrated Electrocatalytic nESI-MS Reaction Platform for In-situ Oxidation of C=C and C=O Bonds**; <u>Kavyasree Chintalapudi</u>; *The Ohio State University, Columbus*

TP 268   **Integrated Simulation of Rarefied Gas Dynamics and Ion Transport with a DSMC Method**; <u>Robin Hillen</u>[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 269   **Paperspray mass spectrometry - A novel technique for the detection of polar compounds in sports drug testing? (A pilot study)**; <u>Christian Görgens</u>[1]; Katherine Walker[2]; Cornelia Boeser[2]; Neloni Wijeratne[2]; Claudia Martins[2]; Sven Guddat[1]; Mario Thevis[1, 3]; *[1]Institute of Biochemistry, German Sport University Cologne, Cologne, Germany; [2]Thermo Fisher Scientific, San Jose, CA; [3]European Monitoring Center for Emerging Doping Agents (EuMoCEDA), Cologne/Bonn, Germany*

TP 270   **A Channel Electron Multiplier Based Ionization Source**; Ely Driscoll[1]; <u>Stephen Ritzau</u>[2]; *[1]University of Connecticut, Storrs, CT; [2]Photonis USA, Inc., Sturbridge, MA*

TP 271   **Non-intrusive Tracking of Drugs of Abuse on Mail/Packaging Using Open Port Interface-Mass Spectrometry**; <u>Haidy Metwally</u>[1]; Prashant Agrawal[1]; Rachael Smith[1]; Chang Chang Liu[2]; Yves Leblanc[2]; Thomas R. Covey[2]; Richard Oleschuk[1]; *[1]Queen's University, Kingston, ON; [2]SCIEX, Concord, ontario*

TP 272   **Acoustic Droplet Ejection from Phase-Separated Liquid Extractions for High-Throughput Mass Spectrometry**; <u>Lucien Ghislain</u>[1]; Chang Liu[2]; Eric Hall[1]; Thomas R Covey[2]; Xiujuan Wen[3]; Kiersten Tovar[3]; Sammy S Datwani[1]; David G Mclaren[3]; *[1]Beckman Coulter Life Sciences, San Jose, CA; [2]SCIEX, Concord, ontario; [3]Merck & Co., Kenilworth, NJ*

TP 273   **Investigation of a fast and versatile analysis platform for screening and quantitation of explosives**; Markus Weber[1]; <u>Jan-Christoph Wolf</u>[2]; Mario F. Mirabelli[3]; *[1]TU Munich, Munich, Germany; [2]Plasmion GmbH, Augsburg, Germany; [3]CTC Analytics AG, Zurich, Switzerland*

TP 274   **Mechanism of Superoxide Adduct Formation in LDTD Ion Source Used in Quantitation**; <u>Pierre Picard</u>[1]; Francis Brière[2]; Sylvain Letarte[1]; Jean Lacoursière[1]; Serge Auger[1]; *[1]Phytronix Technologies, Inc., Quebec, QC; [2]Université Laval, Quebec, Quebec*

TP 275   **Fluid Dynamic and Operational Considerations for an Acoustic Ejection Mass Spectrometry (AEMS) System for High Throughput Analysis**; <u>Chang Liu</u>[1]; Peter Kovarik[1]; Thomas R Covey[1]; *[1]SCIEX, Concord, ON*

TP 276   **Design and Evaluation of a Tethered, Handheld Sampling Probe for Liquid Extraction-Mass Spectrometry Analysis**; <u>Courtney Walton</u>[1]; John F. Cahill[1]; Vilmos Kertesz[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 277   **Dual Capillary-based Vibrating Sharp-edge Spray Ionization (cVSSI) with in-line Hydrogen Deuterium Exchange Mass Spectrometry**; <u>Anthony Debastiani</u>[1]; Sandra N Majuta[1]; Chong Li[1]; Peng Li[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown*

TP 278   **Simulations of Collision Induced Evaporation Processes of Nanodroplets in MS Inlet Stages**; <u>Clara Markert</u>[1]; Walter Wißdorf[1]; Thorsten Benter[1]; Hendrik Kersten[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 279   **Vibrating Sharp-edge Spray Ionization (VSSI) for Direct Analysis of Surface Samples using Mass Spectrometry**; <u>Nandhini Ranganathan</u>[1]; Austin M. Lozier[1]; Michael C. Rawson[1]; Matthew B. Johnson[1]; Stephen J. Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

ION MOBILITY: GENERAL
TP 280-296

TP 280   **Increasing the Resolution of Ion Mobility Separations with Broadly Applicable Ion/Ion Reagents**; <u>Ritu Chaturvedi</u>[1]; Ian Webb[1]; *[1]Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN*

TP 281   **A Modular Machine Learning-Based, Multi-Chemical Class CCS Prediction Pipeline**; Valentin Ianchis[1]; Marisa Gioioso[2]; <u>Joanne Ballantyne</u>[3]; Johannes P.C. Vissers[3]; *[1]Waters Corporation, Brasov, Romania; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 282   **Concurrent Ion Accumulation and Ion Mobility Spectrometry for Increased Ion Utilization**; <u>Ailin Li</u>[1]; Gabe Nagy[1]; Isaac K. Attah[1]; Christopher R. Conant[1]; Adam L. Hollerbach[1]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; Sandilya V. B. Garimella[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 283   **A Fast Scanning Portable Differential Mobility Analyzer Incorporating a CTIA Detector**; <u>Kent Gillig</u>[1]; Da-Shung Su[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

TP 284   **Towards automation of Collision Induced Unfolding experiments through online Size Exclusion Chromatography coupled to native Mass Spectrometry**; <u>Evolène Deslignière</u>[1]; Anthony Ehkirch[1]; Thomas Botzanowski[1]; Oscar Hernandez-Alba[1]; Alain Beck[2]; Sarah Cianférani[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; [2]IRPF, Centre d'Immunologie Pierre Fabre, St-Julien en Genevois, France*

TP 285   **Development of a high resolution Ion Mobility method and its application in prostate cancer metabolism**; Sumankalai Ramachandran[1]; Minas Sakellakis[2]; Christopher Logothetis[1, 3]; Mark Titus[1]; [1]*MD Anderson Cancer Center, Houston, TX;* [2]*Metropolitan Hospital, Neo Faliro, Greece;* [3]*University of Athens, Athens, Greece*

TP 286   **Practical High Resolution Ion Mobility Mass Spectrometry Analyses with Structures for Lossless Ion Manipulations**; John Daniel DeBord[1]; Kelly L Wormwood Moser[1]; Jim Arndt[1]; Nathan Roehr[1]; Liulin Deng[1]; Gordon Anderson[2]; [1]*MOBILion Systems Inc., Chadds Ford, PA;* [2]*GAA Custom Electronics, LLC, Richland, Washington*

TP 287   **A Prototype SLIM-based Ion Mobility Instrument for High Resolving Power Separations Integrated with MS**; Jody C. May[1]; Katrina L. Leaptrot[1]; Bailey S. Rose[1]; Kelly L. Wormwood Moser[2]; Daniel Dubord[2]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Mobilion Systems, Inc., Chadds Ford, PA*

TP 288   **Characteristics analysis of modified oligonucleotides by ion mobility-mass spectrometry (IM-MS)**; Shogo Omuro[1]; Takao Yamaguchi[1]; Taiji Kawase[2]; Maki Terasaki[3]; Kenji Hirose[3]; Satoshi Obika[1]; [1]*Graduate School of Pharmaceutical Sciences, Osaka University, 1-6 Yamadaoka, Suita, Japan;* [2]*Nihon Waters KK, Kitashinagawa, Japan;* [3]*Nihon Waters KK,, Kitashinagawa, Japan*

TP 289   **Probing Protein Structural and Conformational Heterogeneity using Multiplexed Ion Mobility, High Resolution Mass Analysis, and Ultraviolet Photodissociation**; James Sanders[1]; Jamie P. Butalewicz[1]; Sarah N. Sipe[2]; Virginia K. James[2]; Brian H Clowers[3]; Jennifer S. Brodbelt[2]; [1]*University of Texas, Austin, Austin, TX;* [2]*University of Texas Austin, Austin, TX;* [3]*Washington State University, Pullman, WA*

TP 290   **Flowing Atmospheric-Pressure Afterglow Drift Tube Ion Mobility Spectrometry**; Mohsen Latif[1]; Gerardo Gamez[1]; [1]*Texas Tech University, Lubbock, TX*

TP 291   **Implementation and evaluation of electron capture dissociation (ECD) on a cyclic IMS enabled mass spectrometer**; Joseph S. Beckman[1, 2]; Valery G. Voinov[2]; Darren Hewitt[3]; Jason Wildgoose[4]; Jonathan P. Williams[5]; Jeffrey M. Brown[4]; James I Langridge[4]; Dale A. Cooper-Shepherd[4]; [1]*Oregon State University, Corvallis, OR;* [2]*e-MSion, Inc., Corvallis, OR;* [3]*Waters Corporation, Wilmslow, United Kingdom;* [4]*Waters Corporation, Wilmslow, United Kingdom;* [5]*e-MSion Inc., Corvallis, Oregon*

TP 292   **Breaking Down Structural Diversity for Comprehensive Collision Cross Section Prediction Using Machine Learning**; Dylan H Ross[1]; Jang Ho Cho[1]; Libin Xu[1]; [1]*Department of Medicinal Chemistry, University of Washington, Seattle, WA*

TP 293   **The Effect of Solution Conditions on the Collisional Cross Section of GroEL**; Joanna K Denton[1]; Jacob W. McCabe[1]; Christopher S. Mallis[1]; John M. Gordon[1]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX*

TP 294   **Multiplexed Separations for Enhanced Duty Cycle Using Structures for Lossless Ion Manipulations**; Brian H. Clowers[1]; Elvin Cabrera[1]; Liulin Deng[2]; Kelly Moser[2]; Gregory Van Aken[2]; John Daniel DeBord[2]; [1]*Washington State University, Pullman, WA;* [2]*MOBILion Systems Inc., Chadds Ford, PA*

TP 295   **SLIM-QQQ Integration: Coupling High Resolution Mobility Separations with High Sensitivity Mass Analysis for a Next Generation Approach to Quantitative Analysis**; Liulin Deng[1]; Nathan Roehr[1]; Gordon Anderson[2]; Daniel Debord[1]; [1]*MOBILion Systems Inc., Chadds Ford, PA;* [2]*GAA Custom Electronics, LLC, Richland, Washington*

TP 296   **Cyclic ion mobility spectrometry coupled to high-resolution mass spectrometry — Prospects for complex mixture analysis**; Christopher Paul Rüger[1, 2]; Johann Le Maître[2, 3]; Martin Palmer[4]; Eleanor Riches[4]; Carlos Afonso[2, 5]; Pierre Giusti[2, 3]; [1]*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany;* [2]*International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France;* [3]*Total Refining and Chemicals, Harfleur, France;* [4]*Waters Corporation, Wilmslow, United Kingdom;* [5]*University of Rouen-Normandy, Mont-Saint-Aignan, France*

ION MOBILITY: STRUCTURE
TP 297-322

TP 297   **Correlating Gas-Phase Unfolded Conformations To In-Solution Structures Using Single-and Multi-Stage Ion-Mobility and Gas-Phase Simulations**; Charles Eldrid[1]; Tristan Cragnolini[1, 2]; Aisha Ben-Younis[1]; Junjie Zou[3]; Daniel Raleigh[1, 3]; Konstantinos Thalassinos[1]; [1]*University College London, London, United Kingdom;* [2]*Birckbeck, London, United Kingdom;* [3]*Stonybrook University, Stonybrook, NY*

TP 298   **Peptide structure confirmation based on molecular weight and collision cross section obtained with**; Stuart Pengelley[1]; Thomas Schmitz[2]; Diana Imhof[2]; Detlev Suckau[1]; [1]*Bruker Daltonics, Bremen, Germany;* [2]*University Bonn, Protein Synthesis & Bioanalytics Core Facility, Bonn, Germany*

TP 299   **Lipid Isomer Separations via a High Resolution Prototype SLIM-based Ion Mobility Instrument in Support of High Confidence Lipidomics**; Katrina L. Leaptrot[1]; Bailey S. Rose[1]; Jody C. May[1]; Kelly L. Wormwood Moser[2]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Mobilion Systems, Inc., Chadds Ford, PA*

TP 300 **Trapped Ion Mobility Spectrometry (TIMS) enables differentiation of isobaric N-glycan isomers (by specific collisional cross sections)**; Nicolas Grammel[1]; Max Kraner[1]; Sebastian Kandzia[1]; Romano Hebeler[2]; Christian Albers[2]; [1]*Alvotech Hannover, Hanover, Germany;* [2]*Bruker Daltonics, Bremen, Germany*

TP 301 **Probing the Structural Diversity of Vasopressin, Oxytocin, and other Neuropeptide Analogues with Cyclic Multi-Pass Ion Mobility Spectrometry**; Jody C May[1]; Shawn T. Phillips[1]; Emanuel Zlibut[1]; Martin Palmer[2]; James I Langridge[2]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Waters Corporation, Wilmslow, United Kingdom*

TP 302 **Evaluation of Computational Strategies to Interpret Ion Mobility Measurements for Chemically-Diverse Analytes**; Emanuel Zlibut[1]; Berkley Ellis[1]; Jody C. May[1]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN*

TP 303 **Trimethylamine n-Oxide (TMAO) Promotes Substance P Dimer Ions**; Thomas E Walker; *Texas A&M, College Station, TX*

TP 304 **In-depth shape and structural characterisation of complex mixtures of industrial relevance using the SELECT SERIES Cyclic Ion Mobility Mass Spectrometer**; Javeria Mehboob[1]; James Scrivens[1]; Jackie A Mosely[1]; David E Portwood[2]; Pablo Navarro[2]; Martin Palmer[3]; Jakub Ujma[3]; Kevin Giles[3]; [1]*Teesside University, Middlesbrough, United Kingdom;* [2]*SYNGENTA, Bracknell, United Kingdom;* [3]*Waters Corporation, Wilmslow, United Kingdom*

TP 305 **Gas-phase Cross-linking Reactions for Protein Structural Characterization via Ion/Ion Reactions Coupled to Ion Mobility/Time-of-flight Mass Spectrometry**; Melanie Cheung See Kit[1]; Ian K Webb[1]; [1]*Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN*

TP 306 **Complex Dynamic Complexes - The Use of Ion Mobility Mass Spectrometry to Interrogate Protein Structure and Why Charge Matters**; Dale Stuchfield[1]; Jack Roberts[1]; Perdita E Barran[1]; [1]*The University of Manchester, Manchester, United Kingdom*

TP 307 **Structural characterization of polyurethane oligomers and synthetic homopolymers by ion mobility-mass spectrometry**; Kevin M Buck[1]; Rachel A. Harris[1]; Jody C. May[1]; Ian D. Tomlinson[1]; John A. McLean[1]; David M. Hercules[1]; [1]*Vanderbilt University Department of Chemistry, Nashville, TN*

TP 309 **Towards a mechanistic understanding of how glycosylation modulates ligand-binding behavior of ribonuclease using tandem trapped ion mobility spectrometry-mass spectrometry**; Mengqi Chai[1]; Tyler C Cropley[1]; Fanny C. Liu[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

TP 310 **Two-Dimensional Differential/Linear Ion Mobility Separations of Protein Conformations**; Jacob Porter[1]; Alexandre Shvartsburg[2]; Francisco A. Fernandez-Lima[1]; [1]*Florida International University, Miami, FL;* [2]*Wichita State University, Wichita, KS*

TP 311 **Conformational Dynamics of Chaperonin Complexes using nESI-CIA-TIMS-MS**; Kevin Jeanne Dit Fouque[1]; Prem P. Chapagain[1]; Francisco Fernandez-Lima[1]; [1]*Florida International University, Miami, FL*

TP 312 **Challenge of separating 4-dehydroanilinium ion from the radical cation of aniline (the molecular ion) by Ion mobility mass spectrometry**; Athula B. Attygalle[1]; Zhaoyu Zheng[2]; [1]*Stevens Institute of Technology, Hoboken, NJ;* [2]*Stevens Institute of Tecnology, Hoboken, NJ*

TP 313 **Lanthipeptide Topoisomer Screening Based on TIMS-MS/MS**; Kevin Jeanne Dit Fouque[1]; Tung T. Le[2]; Julian D. Hegemann[3]; Wilfred Van Der Donk[2]; Francisco Fernandez-Lima[1]; [1]*Florida International University, Miami, FL;* [2]*University of Illinois at Urbana-Champaign, Urbana, IL;* [3]*Technische Universität Berlin, Berlin, Germany*

TP 314 **Denaturing proteins in ESI droplets: monitoring unfolding transitions by heating differently-sized droplets with a variable-power CO2 laser before IMS-MS analysis**; Shannon Raab[1]; David A. Hales[2]; Wen Liu[3]; Yang Liu[3]; Arthur Laganowsky[3]; David H. Russell[3]; David E. Clemmer[1]; [1]*Indiana University, Bloomington, IN;* [2]*Hendrix College, Conway, AR;* [3]*Texas A&M University, College Station, TX*

TP 315 **The Apparent Density: a critical ion property to consider for ion mobility mass spectrometry analysis**; Christopher Kune[1]; Raphaël La Rocca[1]; Andréa Mc Cann[1]; Jean R. N. Haler[1, 2]; Sophie Rappe[1]; Janina Oetjen[3]; Gauthier Eppe[1]; Johann Far[1]; Edwin De Pauw[1]; [1]*University of Liege, Liège, Belgium;* [2]*Luxembourg Institute of Science and Technology, Belvaux, Luxembourg;* [3]*Bruker Daltonic GmbH, Bremen, Germany*

TP 316 **Native Protein Structural Changes Induced by Exposure to β-Methylamino-L-Alanine as Studied by Ion Mobility-Mass Spectrometry and Collision Induced Unfolding**; Katie Mae Wilson[1]; Samuel W Maddox[1]; Aurora Burkus-Matesevac[1]; Christopher D. Chouinard[1]; [1]*Florida Institute of Technology, Melbourne, FL*

TP 317 **Variable-Temperature Ion Mobility: A 'Cool' Study of IgG Antibody Conformations**; Perdita E Barran[1]; Emma Norgate[1]; [1]*University of Manchester, Manchester, United Kingdom*

TP 318 **Cyclic Ion Mobility– Slice-Collision Activation and Multi-Pass Experiments Probe Dimerization of Aggregation-Prone IAPP**; Aisha Ben-Younis[1]; Charles Eldrid[1]; Alexander Zhyvoloup[1]; Hannah M. Britt[1]; Daniel Raleigh[1, 2]; Konstantinos Thalassinos[1]; [1]*University College London, London, United Kingdom;* [2]*Stony Brook University, Stony Brook, NY*

TP 319 **Collisional-Induced Unfolding and Dissociation of Streptavidin in Tandem-Trapped Ion Mobility Spectrometry/Mass Spectrometry (Tandem-TIMS/MS)**; Wessley Ferguson[1]; Valentina Rangel[1]; Fanny C Liu[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

TP 320 **Characterization of Energy Deposition in Peptide and Protein Ions in Interface of Tandem Trapped Ion Mobility Mass Spectrometry (Tandem TIMS/MS)**; Valentina Rangel[1]; Fanny C Liu[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

TP 321 **A new ion mobility tandem mass spectrometer for isomer-specific fragmentation and cryogenic IR spectroscopy of glycans**; Lei Yue[1]; Robert P Pellegrinelli[1]; Eduardo Carrascosa[1]; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Thomas R. Rizzo[1]; [1]*EPFL/LCPM, Lausanne, Switzerland*

TP 322 **Analysis of Synthesized Polyethylene Glycol-Based Polyurethane Oligomers Using Ion Mobility-Mass Spectrometry**; Rachel Harris[1]; Kevin M Buck[1]; Sahil Soni[1]; Jaqueline A. Picache[1]; Ian D. Tomlinson[1]; Emanuel Zilbut[1]; Berkley M. Ellis[1]; Jody C. May[1]; John A. McLean[1]; David M. Hercules[1]; [1]*Vanderbilt Unviersity, Nashville, Tennessee*

LC/MS: CHROMATOGRAPHY AND SOFTWARE
TP 323-333

TP 323 **Comprehensive Degradant Identification and Management of Analytical Data in Drug Product Development**; Joe Dimartino[1]; Andrew A. Anderson[1]; Sanjivanjit K. Bhal[1]; [1]*ACD/Labs, Toronto, ON*

TP 324 **Development of an analytical reversed phase column for characterization of intact antibodies using wide pore monolithic silica**; Shigenori Ota[1]; Yuko Yui[1]; Shota Miyazaki[2]; Chiaki Aoyama[1]; Ken Miyashita[1]; Manami Takeda[2]; Shunta Futagami[2]; Tsutomu Sato[1]; [1]*GL Sciences Inc., Saitama, Japan; [2]GL Sciences Inc., Tokyo, Japan*

TP 325 **A Novel Mass Spectrometry Peak Tracking Tool for Analytical Quality by Design Method Development**; Fadi L Alkhateeb[1]; Paul Rainville[1]; Nathan Anderson[1]; [1]*Waters Corporation, Milford, MA*

TP 326 **Peptide retention time prediction for TMT-labeled peptides in 2D LC-MS/MS experiments (HILIC, SCX, high pH RP/low pH RP)**; Benilde Mizero[1]; Carina Villacres[2]; Victor Spicer[2]; Rosa Viner[3]; Julian Saba[4]; Bhavinkumar Patel Patel[5]; Sergei Snovida[5]; Penny Jensen[5]; Andreas Huhmer[3]; Oleg Krokhin[1, 2]; [1]*University of Manitoba/Department of Chemistry, Winnipeg, Manitoba; [2]Manitoba Centre for Proteomics and Systems Biology / Department of Internal Medicine, University of Manitoba, Winnipeg, Canada, Winnipeg, MB; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Mississauga, Ontario; [5]Thermo Fisher Scientific, Rockford, IL*

TP 327 **High Throughput Mass Deconvolution Software to Identify and Quantitate Intended and Mispaired Hetero Ig Bispecific Antibody Molecules**; John Robinson[1]; Hannah B. Catterall[1]; John O. Hui[1]; Iain D. G. Campuzano[1]; [1]*Amgen Inc., Thousand Oaks, CA*

TP 328 **Performance of the VICI Valco TrueNano U/HPLC system and sample preparation workflow for single cell level shotgun proteomics**; Guoting Qin[1]; Rufeng Li[1]; Hong Shao[1]; Qiulin Li[1]; Jennifer Copeland[2]; Martin Brisbin[2]; Hal Barnet[2]; Huamin Cai[2]; Stan Stearns[2]; Chengzhi Cai[1]; [1]*University of Houston, Houston, TX; [2]VICI Valco Instruments Co. Inc., Houston, Texas*

TP 329 **MSAnnotate: an MS/MS assistant in-source metabolite ion annotation method for liquid chromatography tandem mass spectrometry (LC-MSMS) based metabolomics**; Yandong Yin[1]; Zheng-Jiang Zhu[2]; [1]*Interdisciplinary Research Center on Biology and Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China; [2]Interdisciplinary Research Center on Biology and Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China*

TP 330 **Machine learning for retention time prediction. Training on METLIN dataset and transfer to nano-HPLC for illicit drugs identification**; Sergey Osipenko[1]; Inga Bashkirova[1]; Sergey Sosnin[1]; Yury Kostyukevich[1]; Eugene (evgeny) Nikolaev[1]; [1]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

TP 331 **Quantitative Amino Acid analysis in Cell Culture Media Using SWATH® Acquisition**; Zuzana Demianova[1]; Jeff Layne[2]; Brian Rivera[2]; Chad Eichman[2]; Lei Xiong[3]; [1]*Sciex, Brea, CA; [2]Phenomenex, Torrance, CA; [3]SCIEX, Redwood Shores, California 1201*

TP 332 **Improved Performance of Modern MS-Compatible Reversed-Phase/Anion-Exchange Mixed-Mode HPLC Columns**; Thomas H. Walter[1]; Bonnie A. Alden[1]; Melvin Blaze[1]; Cheryl Boissel[1]; Donna Osterman[1]; Amit V. Patel[1]; Mathew Delano[1]; Nicole Lawrence[1]; Jessica Field[1]; Moon Chul Jung[1]; [1]*Waters Corporation, Milford, MA*

TP 333 **Expression proteotomics of Clostridum septicum using LC-MS/MS analysis Dominiak B, Mendes M,A Temple University, Philadelphia, Dempster MS Lab,San Paulo Brazil**; Barbara Dominiak; *Temple University, Philadelphia, PA*

TP 334 **A Unique Procedure for Improving Extraction Recovery from Stored Dried Blood Spot Sample in LC-MS/MS Bioanalytical Methods**; Dawei Zhou[1]; John Ma[1]; Silverio Iacono[2]; Sharon Tong[1]; [1]*WuXi AppTec, Cranbury, NJ; [2]Tomtec Inc, Hamden, CT*

LC/MS: SAMPLE PREPARATION II
TP 334-347

TP 335   **Carboxylate modified magnetic bead (CMMB)-based peptide fractionation enables rapid and robust off-line peptide mixture simplification in bottom-up proteomics**; Weixian Deng[1]; Jihui Sha[1]; James A. Wohlschlegel[1]; [1]*UCLA, Los Angeles, CA*

TP 336   **Bioanalytical challenges with BioChaperone® BC structures to quantify parent and truncated metabolite in rat, dog, rabbit and human plasmas**; Gregoire Harichaux[1]; Jordan Goncalves[1]; Mouhssin Oufir[1]; Remi Thouvignon[2]; Peran Terrier[2]; Segolene Laage[2]; Yann Courbebaisse[2]; Fabrice Viviani[1]; [1]*Oncodesign, Villebon-Sur-Yvette, France;* [2]*ADOCIA, LYON, France*

TP 337   **Accomplishing all new challenges for the β-glucuronidases**; Camila Bernes[1]; Jack Andrews[1]; Jose Luis Callejas[1]; Nicholas Chestara[2]; [1]*Kurabiotech, Puerto Varas, Chile;* [2]*DPX Technologies, Columbia, South Carolina*

TP 338   **Improved peptide recovery during proteolytic digestion of low-level protein samples by a simple modification to the FASP approach**; Jennifer J Hill[1]; Tammy-Lynn Tremblay[1]; [1]*National Research Council Canada, Ottawa, ON*

TP 339   **Digestion efficiency in cartridge and bead-based workflows for bottom-up proteomics**; Jessica L. Nickerson[1]; Alan A. Doucette[1]; [1]*Dalhousie University, Halifax, NS*

TP 340   **Micro extraction and LC-MS/MS analysis of multi-class pharmaceutical compounds in human plasma using Solid Phase Extraction Tips**; Mana Shafaei[1]; Kaynoush Naraghi[1]; Corentin Germain[1]; Sami Bayoudh[1]; Raphael Durand[1]; Michel Arotcarena[1]; [1]*AFFINISEP, Petit Couronne, France*

TP 341   **Simplified Sample Preparation for Drugs of Abuse Extraction from Urine Samples Prior to LC-MS/MS Analysis**; Geoff Davies[1]; Lee Williams[1]; Rhys Jones[1]; Katie-Jo Teehan[1]; Adam Senior[1]; Alan Edgington[1]; Helen Lodder[1]; [1]*Biotage GB Limited, Cardiff, United Kingdom*

TP 342   **Optimized Sample Preparation and Off-Line High pH Reversed-Phase Fractionation for TMTpro-labeled Proteomics Samples**; Sergei Snovida[1]; Amarjeet Flora[1]; Ryan Bomgarden[1]; John C Rogers[1]; [1]*Thermo Fisher Scientific, Rockford, IL*

TP 343   **Ultra-Fast Analysis of Nitrosamines Using SPE-QQQ**; Kevin Truempi[1]; Kevin Mccann[1]; [1]*Agilent Technologies, Santa Clara, CA*

TP 344   **Less is more: Avoiding artificial modifications in proteomic sample preparation for pharmaceutical and clinical applications**; Katrin Hartinger[1]; Sebastian H. Johansson[1]; Nils A. Kulak[1]; Katharina Scheck[1]; Fabian Hosp[1]; [1]*PreOmics GmbH, München, Germany*

TP 345   **Fully Automated Sample Preparation Platform for Peptide Mapping and Protein Identification by Mass Spectrometry**; Jia Tang[1]; Yi Zeng[1]; Billy Newton[1]; Guanghui Han[1]; Chri Suh[2]; Rachel Keating[2]; Lee Hoang[2]; [1]*BGI Americas, San Jose, CA;* [2]*PhyNexus now part of Biotage, San Jose, CA*

TP 346   **Low-cost nanoliter pipetting platforms for automated preparation of nanoscale and single-cell proteomic samples**; Yiran Liang[1]; Enoch A. W. Councill[1]; Hayden Acor[1]; Nathanial B. Axtel[1]; Adam L. Aposhian[1]; Thy Truong[1]; Yongzheng Cong[1]; Ying Zhu[2]; Richard H. Carson[1]; Ryan T. Kelly[1, 2]; [1]*Brigham Young University, Provo, UT;* [2]*Pacific Northwest National Laboratory, Richland, WA*

TP 347   **Novel MS compatible surfactant for high temperature protein sample preparation: maximizing protein recovery and digestion efficiency**; Valerie T Ressler[1]; Sergei Saveliev[1]; Wenhui Zhou[1]; Joel Walker[1]; Jean Osterman[1]; Mike Rosenblatt[1]; Poncho Meisenheimer[1]; Marjeta Urh[1]; [1]*Promega Corporation, Madison, WI*

LIPIDS: ID AND STRUCTURAL ANALYSIS
TP 348-370

TP 348   **Unsaturation Elements and other Modifications of Phospholipids in Bacteria: New Insight from UVPD Mass Spectrometry**; Molly S. Blevins[1]; Virginia K. James[1]; Carmen M. Herrera[2]; Alexandria B. Purcell[2]; M. Stephen Trent[2]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*University of Georgia, Athens, GA*

TP 349   **Double bond localization in unsaturated FAME by CI-MS/MS collisional dissociation of acetonitrile adduct [M+40]+**; Zhen Wang[1, 2]; Dong Hao Wang[1, 2]; J. Thomas Brenna[1, 2]; [1]*University of Texas at Austin, Austin, TX;* [2]*Cornell University, Ithaca, NY*

TP 350   **A Simple MALDI/TOF Technique Reveals the Acyl Double-Bond Positions on the Fatty Acyl Coenzyme A Esters**; Hay-Yan J Wang[1]; Fong-Fu Hsu[2]; [1]*National Sun Yat-Sen University, Kaohsiung, Taiwan;* [2]*Washington University in St. Louis, Saint Louis, MO*

TP 351   **Integrating Qual/Quan Workflows for Combined Structure Characterization and Quantitation of Vinyl Ether Phosphatidylethanolamine**; Yulemni Morel[1]; Chinmoy Sarkar[2]; Maureen A Kane[1]; Marta Lipinski[2]; Jace W.

Jones[1]; [1]*University of Maryland, Baltimore School of Pharmacy, Baltimore, MD; [2]University of Maryland, School of Medicine, Baltimore, MD*

TP 352 **4D-Lipidomics investigation in search of the fountain of youth**; Aiko Barsch[1]; Sven W. Meyer[1]; Ulrike Schweiger-Hufnagel[1]; Philippe Schmitt-Kopplin[2, 3]; Michael Witting[2, 3]; [1]*Bruker Daltonics, Bremen, Germany; [2]Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, Neuherberg, Germany; [3]Chair of Analytical Food Chemistry, TU München, Weihenstephan, Germany*

TP 353 **Imaging and Structural Analysis of Fatty Acids in Tissue via Reactive DESI-UVPD-MS**; Luis A Macias[1]; Clara L. Feider[1]; Livia S. Eberlin[1]; Jennifer S. Brodbelt[1]; [1]*University of Texas - Austin, Austin, TX*

TP 354 **Comprehensive analysis of liamocin biosurfactants by means of LC-MS**; Karen Scholz[1]; Till Tiso[2]; Heiko Hayen[3]; [1]*University of Münster - Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]RWTH Aachen University, iAMB - Institute of Applied Microbiology, ABBt – Aachen Biology and Biotechnology, Aachen, Germany; [3]Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

TP 355 **Preferential formation of cationized sphingolipids as protonated sodium salts under ESI conditions yielding fragmentation through proton-driven mechanisms**; Alexandre Seyer[1]; Benoit Colsch[2]; Annelaure Damont[2]; Sylvain Dechaumet[1]; Christophe Junot[2]; François Fenaille[2]; Jean-Claude Tabet[3]; [1]*MedDay Pharmaceuticals, Paris, France; [2]2.   Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), Gif sur Yvette, France; [3]UPMC-CEA, Morangis, France*

TP 356 **Analysis of bacterial lipids using 13C-TrEnDi derivatization and ultraviolet photodissociation mass spectrometry**; Molly S. Blevins[1]; Samuel W Shields[1, 2]; Jeffrey C Smith[2]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX; [2]Carleton University, Ottawa, ON*

TP 358 **Deploying ozone-induced dissociation for targeted and untargeted lipidomic workflows reveals hidden isomeric complexity**; Berwyck Poad[1]; Adam M King[2]; Christopher R. Douglas[1]; Reuben S. E. Young[1]; Martin Green[2]; Lee A Gethings[2]; Todd W Mitchell[3]; Stephen J. Blanksby[1]; [1]*Queensland University of Technology, Brisbane, Australia; [2]Waters Corporation, Wilmslow, United Kingdom; [3]University of Wollongong, Wollongong, Australia*

TP 359 **Automated annotation of FA unsaturation after mCPBA derivatization with LipidSearch and its Lipidomic application using LC with High-resolution Orbitrap MSn**; Daniel Gachotte[1]; Yelena Adelfinskaya[2]; Jeff Gilbert[2]; Ralf Tautenhahn[3]; Yasuto Yokoi[4]; [1]*Corteva, Indianapolis, IN; [2]Corteva Agriscience, Indianapolis, IN; [3]ThermoFisher Scientific, San Jose, CA; [4]Mitsui Knowledge Industry, Tokyo, Japan*

TP 360 **High-Throughput Electron Impact Excitation of Ions from Organics (EIEIO) LC-MS for In-Depth Structural Characterization of Lipids in Complex Mixtures**; Eva Duchoslav[1]; Pavel Ryumin[2]; Jason Causon[2]; Takashi Baba[1]; [1]*SCIEX, Concord, ON; [2]SCIEX, Concord, ontario*

TP 361 **Fatty Acid Structural Elucidation by Pairing the Paternò–Büchi Reaction with Gas-phase Ion/Ion Chemistry using Tris-Phenanthroline Earth Metal Reagents**; De'shovon M. Shenault[1]; Elissia T. Franklin[1]; Scott A. Mcluckey[1]; [1]*Purdue University, Lafayette, IN*

TP 362 **From Static Electricity to Structure: Triboelectric Nanogenerators for Unsaturated Lipid Double Bond Pinpointing**; Marcos Bouza Areces[1]; Yafeng Li[1]; Changsheng Wu[1]; Hengyu Guo[1]; Zhong L. Wang[1, 2]; Facundo M. Fernandez[1]; [1]*Georgia Institute of Technology, Atlanta, GA; [2]Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing,China, China*

TP 363 **Enhancement of Glycerolipid Identification by Pairing Thiol-ene Click Chemistry with Gas-Phase Ion-Ion Reactions**; Elissia Franklin[1]; De'shovon M Shenault[1]; Scott A. Mcluckey[1]; [1]*Purdue University, West Lafayette, IN*

TP 364 **LiPydomics: A Python Package for Analysis of Multi-Dimensional Lipidomics Data and Comprehensive Prediction of Lipid Collision Cross Sections**; Dylan H Ross[1]; Jang Ho Cho[1]; Rutan Zhang[1]; Emily L Pruitt[2]; Libin Xu[1]; [1]*Department of Medicinal Chemistry, University of Washington, Seattle, WA; [2]Department of Chemistry, University of Washington, Seattle, WA*

TP 365 **Gangliosidomics - Identification and screening of gangliosides in mouse brain cortex using ultra-performance liquid chromatography high-resolution mass spectrometry (UPLC-MSE)**; Mona Khorani[1]; Jeffrey Morre[1]; Armando Alcazar Magana[1]; Claudia Susanne Maier[1]; [1]*Department of Chemistry, Oregon State University, Corvallis, Oregon 97331*

TP 366 **Construction of novel lipidomics workflow using TMT derivatization and LipidSearch5.0**; Yasuto Yokoi[1]; Suzumi M Tokuoka[2]; Megumi Ishibashi[3]; Yoshiya Oda[2]; [1]*Mitsui Knowledge Industry Co., Ltd., Tokyo, Japan; [2]The University of Tokyo, Graduate School of Medicine, Lipidomics Laboratory, Tokyo, Japan; [3]Thermo Fisher Scientific, Kanagawa, Japan, Yokohama, Japan*

TP 367 **On-Demand Electrochemical Strategies in Mass Spectrometry for Lipid Analysis**; Shuli Tang[1]; Heyong Cheng[1, 2]; Xin Yan[1]; [1]*Texas A&M University, College Station, TX; [2]Hangzhou Normal Univerisity, Hangzhou, China*

TP 368 **New tools for an advanced 4D-Lipidomics annotation workflow**; Sven Myer[1]; Ansgar Korf[1]; Aiko Barsch[1]; Florian Zubeil[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany*

TP 369 **High-confidence analysis of sphingolipids: integration of off-line LC with high resolution tandem mass spectrometry**; Anh Q. Tran[1]; Jace W. Jones[1]; [1]*University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD*

TP 370 **Online two-dimensional liquid chromatography and high-resolution mass spectrometry for sensitive analysis of cardiolipins and their oxidation products**; Patrick Olaf Helmer[1]; Carina Maria Wienken[1]; Heiko Hayen[1]; [1]*University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

METABOLOMICS: GENERAL I
TP 371-387

TP 371 **Calibrating nonlinear ESI responses using quality control samples to overcome quantitative errors in mass spectrometry-based metabolomics**; Huaxu Yu[1]; Shipei Xing[1]; Lorenz Nierves[1]; Philipp Lange[1]; Tao Huan[1]; [1]*The University of British Columbia, Vancouver, BC*

TP 372 **Combined Quantitation and Profiling Metabolomics to Characterize Laron and Guevara-Rosenbloom Syndromes**; Vanessa Y. Rubio[1]; Clive H. Wasserfall[1]; Jaime Guevara[2]; Mark Atkinson[1]; Arlan Rosenbloom[1]; Alexandra Guevara[3]; Richard A Yost[1]; Timothy J. Garrett[1]; [1]*University of Florida, Gainesville, FL; [2]Universidad San Francisco de Quito, Quito, Ecuador; [3]Instituto de Endocrinologia y Metabolismo, IEMYR, Quito, Ecuador*

TP 373 **Race-specific metabolic landscape identifies altered mitochondrial metabolism in Bladder Cancer**; Karthik Reddy Kami Reddy[1]; Junyoung Park[1]; Roshan Borkar[1]; Ravi Shiva Shankar[1]; Charles Christy[1]; Vasanta Putluri[1]; Benny Abraham Kaipparettu[1]; Jay C Dunn[2]; Patricia D Castro[1]; Michael M Ittmann[1]; Piyarathna Danthasinghe Waduge[1]; Martha K Terris[3]; Stephen B William[4]; Arun Sreekumar[1]; Roni J Bollag[3]; Seth P Lerner[1]; Nagireddy Putluri[1]; [1]*Baylor College of Medicine, Houston, TX; [2]Agilent Technologies, Santa Clara, CA; [3]Augusta Universuty, Augusta, GA; [4]UTMB, Galveston, TX*

TP 374 **Fractionation of metabolites secreted from human microbiota for identification of novel AhR agonists by LC-MS/MS**; Huidi Tian[1]; Lei Wang[1]; Rachel Hardy[2]; Julia Oh[2]; Derya Unutmaz[2]; Xudong Yao[1]; [1]*Department of Chemistry, University of Connecticut, Storrs, CT; [2]Jackson Laboratory for Genomic Medicine, Farmington, CT*

TP 375 **Drugs Purchased on the Surface Web: Untargeted Mass Spectrometry and Molecular Networking Revealed What We Actually Bought**; Kunyang Sun[1]; Alan K. Jarmusch[2]; Aileen Lu[1]; Shaden E. Aguirre[1]; Qing Xu[3]; Timothy K. Mackey[3, 4, 5]; Pieter C. Dorrestein[2, 6, 7]; [1]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences and Collaborative Mass Spectrometry Innovation Center, University of California, San Diego, La Jolla, 92093; [3]Department of Healthcare Research and Policy, University of California, San Diego - Extension, La Jolla, CA; [4]Department of Anesthesiology, University of California, San Diego - School of Medicine, La Jolla, CA; [5]Global Health Policy Institute, San Diego, La Jolla, CA; [6]Department of Pediatrics, University of California, San Diego, La Jolla, CA; [7]Center for Microbiome Innovation, University of San Diego, La Jolla, CA*

TP 376 **Mass Spectrometry Study of Carnitine Vs. Benznidazole in Acute Stage Chagas Disease Treatment**; Ekram Hossain[1]; Danya A Dean[1]; Laura-Isobel Mccall[1]; Mitchelle Katemauswa[1]; Stephanie Hayes[1]; Lindise Martin[1]; Yiming Zhang[1]; Shelly S Kane[1]; [1]*University of Oklahoma, Norman, OK*

TP 377 **Plasma-Based Metabolomics for Estimating Benchmark Doses of Apical Outcomes**; David M. Crizer[1]; Zhifeng Zhou[1, 2]; William M. Gwinn[1]; Scott S. Auerbach[1]; Michael J. Devito[3]; B. Alex Merrick[1]; [1]*National Toxicology Program/NIEHS/NIH, Research Triangle Park, NC; [2]School of Public Health, Southern Medical University, Guangzhou, China; [3]US Environmental Protection Agency, Office of Research and Development, Research Triangle Park, NC*

TP 378 **Sebum : a window into dyregulation of lipids and energy metabolism in Parkinson's disease**; Drupad K Trivedi[1]; Eleanor Sinclar[2]; Depanjan Sarkar[2]; Caitlin Walton-Doyle[2]; Joy Milne[2]; Tilo Kunath[3]; Anouk M Rijs[4]; Rob De Bie[5]; Roy Goodacre[6]; Monty Silverdale[2]; Perdita E Barran[1]; [1]*University of Manchester, Manchester, United Kingdom; [2]The University of Manchester, Manchester, United Kingdom; [3]University of Edinburgh, Edinburgh, United Kingdom; [4]Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Nijmegen, Netherlands; [5]Amsterdam UMC, Amsterdam, Netherlands; [6]University Of Liverpool, Liverpool, United Kingdom*

TP 379 **Robust metabolomics workflows using a modified benchtop Orbitrap Mass Spectrometer**; Mark J Schroeder[1]; Ioanna Ntai[1]; Tatjana Talamantes[1]; Siegrun Mohring[2]; Markus Kellmann[2]; Alexander Harder[2]; Ralf Tautenhahn[1]; Amanda Souza[1]; Andreas Huhmer[1]; [1]*Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 380 **Metabolic adaptation analysis of the inhibition of oxidative phosphorylation using time-series metabolomics and lipidomics**; Nobuyuki Okahashi[1]; Shuma Tsuji[1]; Junko Iida[1, 2]; Tairo Ogura[2]; Fumio Matsuda[1]; [1]*Osaka University, Osaka, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

TP 382   **Characterization of Gut-Brain Axis Communication of Tryptophan Metabolites Using UHPLC-HRMS**; Richard C Dilworth[1]; Vanessa Y. Rubio[2]; Gary P Wang[2]; Richard A Yost[2]; Timothy J Garrett[2]; [1]*University of Florida, Gainesville, FL;* [2]*University of Florida, Gainesville*

TP 383   **Metabolomics in the tissue engineer's toolbox: defining unique biological processes in neurogenesis cued by soluble or immobilized IFN γ**; Hannah Baumann[1]; Nic D Leipzig[1]; Leah P Shriver[1]; [1]*University of Akron, Akron, OH*

TP 385   **On the Origin of Protons in Electrospray Ionization**; Yixin Zhu[1]; Kai Tang[1]; [1]*Zhejiang Haochuang Biotech Co. Ltd., Hangzhou, China*

TP 386   **Merging untargeted and targeted analysis of the lipidome, metabolome, and exposome**; Tomas Cajka[1]; Jiri Hricko[1]; Michaela Novakova[1]; Michaela Paucova[1]; Ondrej Kuda[1]; [1]*Institute of Physiology CAS, Prague, Czech Republic*

TP 387   **Evaluation of LC-MS mobile-phase modifiers for metabolomic and lipidomic profiling**; Jiri Hricko[1]; Tomas Cajka[1]; Michaela Paucova[1]; Michaela Novakova[1]; [1]*Institute of Physiology CAS, Prague, Czech Republic*

METABOLOMICS: IDENTIFICATION OF UNKNOWN METABOLITES
TP 388-403

TP 388   **Compound identification strategies in metabolomics: What if MS/MS is not enough?**; Charles R Evans[1]; Brady G Anderson[1]; Alla Karnovsky[1]; Hani Habra[1]; Maureen T Kachman[1]; Alexander B Raskind[1]; [1]*University of Michigan, Ann Arbor, MI*

TP 389   **Expanding coverage and confidence of metabolites in Cancer cells by cross-validations using targeted and untargeted approaches with open source tools**; Li Zhang[1]; Anthony Andren[2]; Costas Lyssiotis[3]; [1]*University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan;* [2]*University of Michigan School of Medicine, Rogel Cancer Center, Ann Arbor, Michigan;* [3]*University of Michigan, School of Medicine, Rogel Cancer Center, Ann Arbor, Michigan*

TP 390   **Isomeric Differentiation and Acidic Metabolite Identification by basic Tagging, LC-MS/MS, and Understanding of the Dissociation Chemistries**; Shanshan Guan[1, 2]; Michael R. Armbruster[3]; James L. Edwards[3]; Benjamin J Bythell[1, 2]; [1]*Ohio University, Athens, OH;* [2]*University of Missouri, St. Louis, St. Louis, MO;* [3]*Saint Louis University, Saint Louis, MO*

TP 392   **Unraveling the chemical nature of biofluids by using reference materials, ARUS libraries and the hybrid search. Do it yourself**; Yamil Simón-Manso[1]; Xinjian Yan[1]; Kelly H. Telu[1]; Yuri A. Mirokhin[1]; Yuxue Liang[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

TP 393   **Untargeted Screening in a Case Control Study Using Apples as a Matrix**; Erica L Bakota[1]; Robert A Levine[1]; [1]*U.S. Food and Drug Administration, Lenexa, KS*

TP 394   **Development of a suite of machine learning-based models for large-scale prediction of collisional cross sections of natural products**; Skyler T. Kramer[1, 2]; Feng Qiu[1, 2, 3]; Barbara W Sumner[1, 2]; Sean M. Colby[4]; Ryan S. Renslow[4]; Thomas O. Metz[4]; Lloyd W. Sumner[1, 2]; [1]*Department of Biochemistry, University of Missouri, Columbia, MO;* [2]*University of Missouri Metabolomics Center, Columbia, Missouri;* [3]*International Flavor and Fragrance, Union Beach, NJ;* [4]*Pacific Northwest National Lab, Richland, WA*

TP 395   **Metabolite Profiling of Centella asiatica L. Leaves using Ultrahigh Resolution Fourier Transform Ion Cyclotron Mass Spectrometry**; Syful Islam[1, 2]; Sunghwan Kim[1, 3]; [1]*Department of Chemistry, Kyungpook National University, Daegu, South Korea;* [2]*Department of Environment, Munshiganj District Office, Munshiganj, Bangladesh;* [3]*Green-Nano materials Research Center, Daegu, South Korea*

TP 396   **Unravelling via Mass Spectrometry the L-Argininosuccinic acid cyclization in biological samples**; Ana Gradillas[1]; Maricruz Mamani-Huanca[1]; Ángeles López-Gonzálvez[1]; Coral Barbas[1]; [1]*CEMBIO, Universidad CEU San Pablo, Boadilla del Monte, Spain*

TP 397   **Metabolite identification by assignment of collisional-cross section (CCS) and isotopic fine structure (IFS)**; Joel Gummer[1]; Nathan Lawler[1]; Berin Boughton[1]; Melvin C.L. Gay[2]; Samantha Lodge[1, 3]; Christopher Thompson[4]; Elaine Holmes[1, 5]; Jeremy Nicholson[1, 3]; [1]*Australian National Phenome Centre, Murdoch University, Murdoch, Australia;* [2]*Bruker Pty Ltd, Preston, Australia;* [3]*Health Futures Institute, Murdoch University, Murdoch, Australia;* [4]*Bruker Daltonics, Billerica, MA;* [5]*Research and Innovation Office, Murdoch University, Murdoch, Australia*

TP 398   **MetFID: Metabolite Annotation Using Artificial Neural Network**; Ziling Fan[1]; Amber Alley[1]; Kian Ghaffari[1]; Habtom Ressom[1]; [1]*Georgetown University, Washington, DC*

TP 399   **Identifying plant natural products in the food we eat by untargeted metabolomics**; Arpana Vaniya[1]; Ying Y. Choy[1]; Alberto Valdés[1]; Sajjan Singh Mehta[1]; John de la Parra[2]; Carol D. Stroble[1]; Tong Shen[1]; Luis M. Valdiviez[1]; Michael Sebek[3]; Rebekah Carlson[4]; Caleb Harper[4, 5]; Oliver Fiehn[1]; [1]*West Coast Metabolomics Center, UC Davis, Davis, CA;* [2]*Harvard University Herbaria, Cambridge, MA;* [3]*Center for Complex Network Research, Department of*

Physics, Northeastern University, Boston, MA; [4]Open Agriculture (OpenAg) Foundation, Cambridge, MA; [5]Massachusetts Institute of Technology, Cambridge, MA

TP 400   **MetaboQuest: A Suite of Tools for Metabolite Annotation**; <u>Habtom W Ressom</u>[1]; Linge Yan[1]; Mohammad R Nezami-Ranjbar[1]; [1]*OmicsCraft, Washington, District of Columbia*

TP 401   **Untargeted vs amine targeted metabolomics of MRSA to identify antibiotic agent biomarkers**; <u>Amar Deep Sharma</u>[1]; Nitish R. Mishra[1]; William G. Gutheil[1]; [1]*University of Missouri-Kansas City, Kansas City, MO*

TP 402   **Paired mass distance dependent analysis (PMDDA) for robust untargeted compound identification**; Miao Yu[1]; <u>Lauren Petrick</u>[1]; Georgia Dolios[1]; [1]*Icahn School of Medicine at Mount Sinai, New York, NY*

TP 403   **Analysis of Penillium sclerotiorum specialized metabolome by molecular networking**; Teo Hebra[1]; Veronique Eparvier[1]; <u>David Touboul</u>[1]; [1]*CNRS-ICSN, Institut de Chimie des Substances Naturelles, UPR 2301, Université Paris Saclay, Orsay, France*

MICROORGANISMS AND THE MICROBIOME II
TP 404-421

TP 404   **Robust Accurate Identification and Biomass Estimates of Microorganisms via Tandem Mass Spectrometry**; <u>Gelio Alves</u>[1]; Yi-Kuo Yu[1]; [1]*National Center for Biotechnology Information, NLM, Bethesda, MD*

TP 405   **Metabolomics analysis of colorectal cancer-associated anaerobic bacteria co-cultured with tumor spheroids**; <u>Thomas P Wyche</u>[1]; Stephen H Kasper[1]; Carolina Morell-Perez[1]; Linda A Lieberman[1]; Erik C Hett[1]; Theodore R Sana[1]; [1]*Exploratory Science Center, Merck & Co., Inc., Cambridge, MA*

TP 406   **Identifying heat stress correlated metabolites in reef building corals**; <u>Eric N Chiles</u>[1]; Amanda Williams[2]; Debashish Bhattacharya[2]; Xiaoyang Su[1, 3]; [1]*Metabolomics Shared Resource, Rutgers University, New Brunswick, NJ; [2]Department of Biochemistry and Microbiology, Rutgers University, New Brunswick, NJ; [3]Department of Medicine, Division of Endocrinology, Robert Wood Johnson Medical School, Rutgers University, New Brunswick, NJ*

TP 407   **Fast Lipid Extraction Technique for rapid MALDI-TOF-MS identification of Microbes**; <u>David R Goodlett</u>[1, 2]; Francesca Gardener[3]; Hyojik Yang[3]; Sung Hwan Yoon[4]; Tao Liang[3]; Courtney Chandler[3]; Robert K Ernst[3]; Matthew Sorensen[5]; Erik Nilsson[5]; [1]*University of Maryland, Baltimore, MD; [2]International Centre for Cancer Vaccine Science, Gdansk, Poland; [3]University of Maryland Balitmore, Baltimore, MD; [4]NIH, Bethesda, Maryland; [5]Pataigin, LLC, Baltimore, MD*

TP 408   **Bile Acid Profile and its Changes in Response to Cefoperazone Treatment in MR1 Deficient Mice**; <u>Jinchun Sun</u>[1]; Zhijun Cao[1]; Ashley D. Smith[2]; Paul E. Carlson Jr[3]; Michael Coryell[2]; Huizhong Chen[1]; Richard Beger[1]; [1]*NCTR / USFDA, Jefferson, AR; [2]CBER, Silver Spring, MD; [3]CBER, Silver Spring, MS*

TP 409   **Complex Community Metabolome Interactions from the Cheese Rind-Derived Microbiome**; <u>Gordon T Luu</u>[1]; Jessica Cleary[1]; Emily C Pierce[2]; Rachel J Dutton[2]; Laura M Sanchez[1]; [1]*University of Illinois at Chicago, Chicago, IL; [2]UCSD, La Jolla, CA*

TP 410   **Optimization of protein extraction methods to study root-associated microbes with metaproteomics**; <u>Fernanda Salvato</u>[1]; Clara Tang[2]; Omri Finkel[3]; Jeffery L. Dangl[3]; Ben Niu[4]; Manuel Kleiner[2]; [1]*North Carolina State University, raleigh, NC; [2]North Carolina State University, Raleigh, NC; [3]University of North Carolina at Chapel Hill, Chapel Hill, NC; [4]State Key Laboratory of Tree Genetics and Breeding, Northeast Forestry University, Harbin, China*

TP 411   **Measuring short-chain fatty acids in microbiome-derived samples by LC-MS/MS**; <u>Sigmund J. Haidacher</u>[1, 2]; Thomas D. Horvath[1, 2]; Kathleen M. Hoch[1, 2]; Melinda A. Engevik[1, 2]; Faith D. Ihekweazu[1, 2]; Anthony M. Haag[1, 2]; [1]*Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital - Microbiome Center, Houston, TX*

TP 412   **Extraction Development for Metabolomics Analysis of the Cystic Fibrosis Pulmonary Microbiome**; <u>Brent D Carrillo</u>[1]; Vanessa Phelan[1]; [1]*CU Denver Anschutz Medical Campus, Aurora, CO*

TP 413   **Rapid differentiation of antibiotic-resistant Staphylococcus aureus using secondary electrospray ionization mass spectrometry**; <u>Jiangjiang (chris) Zhu</u>; *The Ohio State University, Columbus, OH*

TP 414   **Biosynthesis pathway of indole-3-acetic acid in Candida tropicalis**; <u>Masaru Miyagi</u>[1]; Christopher L. Hager[1]; Thomas Mccormick[1]; Mahmoud A. Ghannoum[1]; [1]*Case Western Reserve University, Cleveland, OH*

TP 415   **Metaproteomic analysis of murine gut and nasopharyngeal microbiomes in response to infection**; <u>Joby Cole</u>[1, 2, 3]; Caroline Evans[3]; Mark Dickman[3]; [1]*The Florey Institute, Sheffield, United Kingdom; [2]Department of Infection, Immunity & Cardiovascular Diseases, Sheffield, United Kingdom; [3]Department of Chemical and Biological engineering, Sheffield, United Kingdom*

TP 416   **Mapping of bacterial metabolism with stable-isotope labeled tracers and HRAM-LC-MS**; <u>Thomas D. Horvath</u>[1, 2]; Qinglong Wu[1, 2]; Sigmund J. Haidacher[1, 2]; Kathleen M. Hoch[1, 2]; Tor C. Savidge[1, 2]; Anthony M. Haag[1, 2]; [1]*Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital - Microbiome Center, Houston, TX*

TP 417   **LC-MS-MS Identification of Bacteriophage and Host Peptides after CsCl gradient isolation**; Leslie Harden[1]; Yen-Te Liao[1]; Vivian C.H. Wu[1]; *[1]USDA/WRRC, Albany, CA*

TP 418   **Urinary protein deposition and its effect on biofilm formation on urinary catheters by nonpathogenic and pathogenic bacteria**; Rufeng Li[1]; Guoting Qin[1]; Yanxin Chen[1]; Mengfan Wang[1]; Christopher Thang[1]; Chengzhi Cai[1]; *[1]University of Houston, Houston, TX*

TP 419   **Characterization of substrate specificity of Staphylococcus aureus secreted lipases using HILIC-ion mobility-mass spectrometry**; Emily L Pruitt[1]; Tianwei Shen[2]; Rutan Zhang[2]; Dylan H Ross[2]; Xi Chen[3]; Francis Alonzo Iii[3]; Libin Xu[2]; Matthew F. Bush[1]; *[1]Department of Chemistry, University of Washington, Seattle, WA; [2]Department of Medicinal Chemistry, University of Washington, Seattle, WA; [3]Department of Microbiology and Immunology, Loyola University, Chicago, IL*

TP 420   **In-depth structure characterization of lipopolysaccharide via integration of chromatography, ion mobility, and high-resolution tandem mass spectrometry**; Cassandra E Nelson[1]; Eugene Moskovets[2]; Amanda Oglesby-Sherrouse[1]; Jace W Jones[3]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]Mass Tech, Inc., Columbia, MD; [3]University of Maryland, School of Pharmacy, Baltimore, MD*

TP 421   **Mass spectrometry-based mapping of rabbit ocular surface proteome and microbiome**; Guoting Qin[1]; Chengzhi Cai[1]; *[1]University of Houston, Houston, TX*

NANOSCALE AND MICROFLUIDIC SEPARATIONS AND MS
TP 422-426

TP 422   **Combined LC-MS and Microflow 1H NMR strategy for the identification of volume and mass-limited lipid isomers**; Jiajun Lei[1]; Matthew E. Merritt[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

TP 423   **Capillary flow LC-MS using micro pillar array columns: combining nano flow sensitivity with analytical flow robustness and throughput**; Geert Van Raemdonck[1]; Jeff Op De Beeck[1]; Paul Jacobs[1]; Gert Desmet[2]; *[1]PharmaFluidics, Zwijnaarde, Belgium; [2]Vrije Universiteit Brussel, Brussels, Belgium*

TP 424   **A new high-pressure station for the multiplexed packing of capillary columns**; Johannes B Müller[1]; Peter V Treit[2]; Lisa C Schweizer[3]; Philipp E Geyer[2, 4]; Matthias Mann[2, 4]; *[1]Max Planck Institute of Biochemie, Martinsried, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Max Planck Institute of Biochemistry, München, Germany; [4]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark*

TP 425   **µRIPS - Microfludic Refrigeration Induced Phase Separation for ESI-MS Analysis of Complex Biochemical Samples**; Austin L. Culberson[1]; Yichun Zhou[1, 2]; Peter A. Kottke[1]; Andrei G. Fedorov[1, 3]; *[1]The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA; [2]Pratt School of Engineering, Duke University, Durham, NC; [3]Parker H. Petit Institute for Bioengineering & Biosciences, Georgia Institute of Technology, Atlanta, GA*

TP 426   **Analysis of Bioreactor Cell Growth Media with Microchip Capillary Electrophoresis-Negative Electrospray Ionization-Mass Spectrometry**; Yury Desyaterik[1]; Jean P Alarie[1]; Glenn A Harris[2]; Kenion H Blakeman[2]; Ryan R Barton[3]; J. Michael Ramsay[1]; *[1]UNC Chapel Hill, Chapel Hill, NC; [2]908 Devices, Inc., Boston, MA; [3]North Carolina State University, Raleigh, NC*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES I
TP 427-446

TP 427   **Mechanism for the binding of netropsin to hairpin DNA revealed using nanoscale ion emitters in native mass spectrometry**; Giang Nguyen; *University of New South Wales, Sydney, Australia*

TP 428   **Development of UPLC-MS Method for Global RNA Modification Analysis in SaccharomycesCerevisiaemRNAs**; Qishan Lin; *University at Albany, Albany, NY*

TP 429   **A Whole New World: TEA and HFIP free LC-MS conditions for siRNA analysis to enable monitoring of small molecule impurities**; Jennifer Lippens[1]; Shawn Pope[1]; Laura Blue[1]; Tawnya Flick[1]; *[1]Amgen, Thousand Oaks, CA*

TP 430   **Liquid chromatography-based fractionation of eukaryotic transfer RNA for improved RNA modification mapping by LC-MS/MS**; Gwenn G. Parungao[1]; Scott Abernathy[1]; Manasses Jora[1]; Robert Ross[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 431   **Pytheas: a platform for the identification, mapping and statistical analysis of RNA post-transcriptional modifications via LC-MS**; Luigi D'ascenzo[1]; Anna Popova[1]; James R. Williamson[1]; *[1]The Scripps Research Institute, La Jolla, CA*

TP 432   **Evaluation of a new software tool for assisting with the siRNA metabolite identification by LC-MS**; Babak Basiri[1]; Wilfred Tang[2]; Marshall Bern[2]; Yong J Kil[2]; Maria Basanta-Sanchez[2]; Mei Han[1]; Fang Xie[1]; Brooke M. Rock[1]; *[1]Amgen Inc., South San Francisco, CA; [2]Protein Metrics, Cupertino, CA*

TP 433 **A Scheduled LC-MS3Method for Assessing the Epitranscriptome**; <u>Gwendolyn Gonzalez</u>[1]; Yuxing Cui[1]; Yinsheng Wang[1]; Pengcheng Wang[1]; [1]*University of California-Riverside, Riverside, CA/US*

TP 434 **High-throughput Mass Spectrometry Analysis of Synthetic Oligonucleotides: A Comparison of Data from Fast LC and RapidFire Methods**; <u>Peter Rye</u>[1]; Yanan Yang[2]; [1]*Agilent, Lexington, MA; [2]Agilent Technologies, Santa Clara, CA*

TP 435 **"xNA Analyzer": a novel computational tool for characterizing therapeutic oligonucleotides using liquid chromatography-tandem mass spectrometry data**; <u>Yuki Matsubara</u>[1]; Yasuto Yokoi[1]; Masami Koike[2]; Masato Taoka[3]; Yuko Nobe[3]; Hiroshi Nakayama[2]; [1]*Mitsui Knowledge Industry, Tokyo, Japan; [2]RIKEN CSRS, Wako, Japan; [3]Tokyo Metropolitan University., Hachioji, Japan*

TP 436 **Metabolite Profiling and Identification of an Antisense Oligonucleotide (ASO), Deconjugated ASOs, and Chain-Shorted ASOs from Human Plasma using IP-LC-UV-MS**; <u>Dennis Kraus</u>[1]; Noah Post[2]; Shannon Hall[2]; Fumin Li[1]; [1]*PPD, Middleton, WI; [2]Ionis Pharmaceuticals, Inc, Carlsbad, CA*

TP 437 **Understanding retention mechanisms of oligonucleotides during hydrophilic interaction liquid chromatography mass spectrometry**; <u>Scott Abernathy</u>[1]; Peter A. Lobue[1]; Naman Dhingra[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH*

TP 439 **Detection of complex tRNA modifications by mass spectrometry using NucleicAcidSearchEngine**; <u>Samuel P Wein</u>[1]; Byron Andrews[2]; Hendrik Weisser[2]; [1]*University of Tübingen, Tübingen, Germany; [2]Storm Therapeutics, Cambridge, United Kingdom*

TP 440 **A MSMS auto-workflow for synthetic oligonucleotide sequence confirmation**; <u>Walter Wang</u>; *Alnylam, Cambridge, MA*

TP 441 **Deinococcus radiodurans Transfer RNA Modified Nucleosides are Minimally Impacted by UVA Radiation**; <u>Ruoxia Zhao</u>[1]; Spencer Parrish[1]; Robert L. Ross[1]; Manasses Jora[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH*

TP 442 **Quantitative determination of PMOs and PPMOs in mouse and monkey tissues by UPLC-HRMS**; John Chen[1]; Jianbo Zhang[2]; Ran An[1]; Jian Shi[1]; <u>Chengjie Ji</u>[1]; John Hadcock[2]; [1]*Novabioassays LLC, Woburn, MA; [2]Sarepta Therapeutics, Cambridge, MA*

TP 443 **Climbing the oligonucleotide ladder toward rapid and wide-ranging oligonucleotide analysis using benchtop MALDI-MS**; <u>Dominique B Figueroa</u>[1]; Vikki Johnson[1]; M. Nazim Boutaghou[2]; Jordan Frost[1]; [1]*Shimadzu Scientific Instruments, Inc, Carlsbad, CA; [2]Shimadzu Scientific Instruments Inc., Columbia, MD*

TP 444 **LC-MS based analysis of the structural and functional roles of rRNA post-transcriptional modifications under photooxidative stress**; <u>Mariana B. P. Estevez</u>[1]; Manasses Jora[1]; Scott Abernathy[1]; Patrick A. Limbach[1]; Balasubrahmanyam Addepalli[1]; [1]*Rieveschl Laboratories for Mass Spectrometry, University of Cincinnati, Cincinnati, OH*

TP 445 **Informatics-informed polarity-switching LC-MS/MS workflow for annotation of novel modified RNAs**; <u>Rebecca Rose</u>[1]; Olga Katsara[1]; Robert Banh[1]; Tenzin Lhakhan[1]; Manor Askenazi[1]; Robert Schneider[1]; Michael Pacold[1]; Drew Jones[1]; [1]*NYU Langone Health, New York, NY*

TP 446 **Automatic identification of antisense locked nucleic acid by liquid chromatography - tandem mass spectrometry and combinatorial sequence database search**; <u>Kurokawa Yusaku</u>[1]; Matsubara Yuki[1]; Masami Koike[2]; Yoshio Yamauchi[3]; Taoka Masato[3]; Yokoi Yasuto[1]; Nakayama Hiroshi[2]; [1]*Mitsui Knowledge Industry, Tokyo, Japan; [2]RIKEN Center for Sustainable Resource Science, Wako, Japan; [3]Tokyo Metropolitan University., Hachioji, Japan*

PEPTIDES: PTM IDENTIFICATION II
TP 447-461

TP 447 **High throughput fine mapping of glycosylation enabled by DiLeuEN and ETD-MS**; <u>Miyang Li</u>[1]; Lingjun Li[2]; [1]*University of Wisconsin Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

TP 448 **Profiling Tumor Microenvironment-Induced Changes in the Post-Translationally Modified Proteome in KPC Mouse-Derived Pancreatic Cancer Spheroids**; <u>Dylan Nicholas T Tabang</u>[1]; Philip B Emmerich[2, 3]; Yusi Cui[1]; Yuan Liu[4]; Dustin A Deming[2, 3, 5, 6]; Lingjun Li[1, 4]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Division of Hematology and Medical Oncology, Department of Medicine, University of Wisconsin School of Medicine and Public Health, University of Wisconsin, Madison, WI; [3]University of Wisconsin Carbone Cancer Center, Madison, WI; [4]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [5]William S. Middleton Memorial Veterans Hospital, Madison, WI; [6]McArdle Laboratory for Cancer Research, Department of Oncology, University of Wisconsin School of Medicine and Public Health, Madison, WI*

TP 449 **Identification and differentiation of disulfide bonded isomers of the μ-conotoxin PIIIA by trapped ion mobility spectrometry**; <u>Thomas Schmitz</u>[1]; Stuart Pengelley[2]; Eckhard Belau[2]; Diana Imhof[1]; Detlev Suckau[2];

[1]University Bonn, Protein Synthesis & Bioanalytics Core Facility, Bonn, Germany; [2]Bruker Daltonics, Bremen, Germany

TP 450 **Mass spectrometry-based data validation and machine learning models for citrullinome analysis**; Raghothama Chaerkady[1]; Jared Delmar[1]; Wen Yu[1]; Yebin Zhou[1]; Gary P Sims[1]; Lisa H Cazares[1]; Sonja Hess[1]; *[1]R&D AstraZeneca, Gaithersburg, MD*

TP 451 **Retention Time Prediction for Phosphorylated Peptides in 2D HPLC-MS Proteomic Experiments**; Taylor Battellino[1]; Darien Yeung[2]; Ying Lao[3]; Victor Spicer[3]; Helene Perreault[1]; Oleg Krokhin[4]; *[1]University of Manitoba/Department of Chemistry, Winnipeg, Manitoba; [2]University of Manitoba, Winnipeg, MB; [3]Manitoba Centre of Proteomics and Systems Biology, Winnipeg, MB; [4]Manitoba Centre for Proteomics and Systems Biology / Department of Internal Medicine, University of Manitoba, Winnipeg, Canada, Winnipeg, MB*

TP 452 **Leveraging diagnostic ions for targeting acyl-lysine modifications in proteomic datasets**; Janine Fu[1]; John Muroski[1]; Hong Hahn Nguyen[1]; Robert P. Gunsalus[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

TP 453 **A pipeline for localization of post-translational modifications in shotgun proteomics based on statistical assessment of mass shifts of identified peptides**; Julia A. Bubis[1]; Lev I. Levitsky[1]; Mark V. Ivanov[1]; Mikhail V Gorshkov[1]; Irina A. Tarasova[1]; *[1]V.L. Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation*

TP 454 **Automated, Robust, and Sensitive Peptide Ubiquitin-Remnant Enrichment Workflow Applied to Determine Substrates of the E3 ligase Cbl-b**; Jonas Kolibius[1]; David Avila[1]; Martin Ebeling[1]; Tom Dunkley[1]; Christine Hildebrandt[2]; Adrian Britschgi[2]; Manuel Tzouros[1]; *[1]Roche Innovation Center Basel, Pharma Research and Early Development, Pharmaceutical Sciences, F. Hoffmann-La Roche Ltd., Basel, Switzerland; [2]Roche Innovation Center Basel, Pharma Research and Early Development, Oncology Discovery and Translational Medicine Area, F. Hoffmann-La Roche Ltd., Basel, Switzerland*

TP 455 **Ion Mobility Mass Spectrometry of Glyco- and Phospho-Peptides**; Marshall W. Bern[1]; Yong J Kil[1]; Abhishek Roushan[1]; Doron Kletter[1]; Claire J Bramwell[1]; Eric Carlson[1]; Guillaume Tremintin[2]; Christopher Adams[2]; Nagarjuna Nagaraj[2]; *[1]Protein Metrics Inc, Cupertino, CA; [2]Bruker Scientific, San Jose, CA*

TP 456 **A Novel Detection Method for Aspartic Acid Isomerization Using Diagnostic a-Ions in Radical Directed Dissociation Mass Spectrometry**; Evan E Hubbard[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

TP 457 **Leveraging the extended instrument capabilities of a Tribrid MS using real-time PTM localization**; William D Barshop[1]; Jesse D Canterbury[1]; Tony Zhao[1]; Romain Huguet[1]; Vlad Zabrouskov[1]; Graeme Mcalister[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 458 **Assessing oxidation in IgG1 monoclonal antibodies and correlating at both the intact protein and the peptide levels**; Tom Buchanan[1]; Sara Carillo[2]; Angela Criscuolo[3]; Silvia Millan Martin[2]; Jennifer Sutton[4]; Phil J Widdowson[1]; Ken Cook[1]; Kai Scheffler[5]; Jonathan Bones[2]; *[1]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [2]NIBRT, Dublin, Ireland; [3]Thermo Fisher Scientific, Dreieich, Germany; [4]Thermo Fisher Scientific, San Jose, California; [5]Thermo Fisher Scientific, Germering, Germany*

TP 459 **Sequential phosphoproteomics and N-glycoproteomics of plasma-derived extracellular vesicles for breast cancer subtype biosignatures**; Hillary Andaluz Aguilar[1]; I-Hsuan Chen[1]; J. Sebastian Paez[1]; Marco Hadisurya[1]; Anton B Iliuk[2]; Guochen Qin[3]; Haiyang Zhang[4]; Chuan-Chih Hsu[1]; Sujun Li[5]; Jian-Kang Zhu[3]; Sonia Sugg[6]; Michael K. Wendt[1]; Haixu Tang[5]; Weizhou Zhang[7]; W. Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]Tymora Analytical Operations, West Lafayette, Indiana; [3]Shanghai Institute of Plant Stress Biology, Shanghai, China; [4]School of Biological Sciences and Medical Engineering, Southeast University, Nanjing, China; [5]Indiana University, Indianapolis, IN; [6]University of Iowa, College of Medicine, Iowa City, Iowa; [7]University of Florida, Gainesville, FL*

TP 460 **Trapped- Ion Mobility High Resolution QTOF MS - Impact of PASEF and diaPASEF on detection and identification of post-translational modifications**; Allan Stensballe[1]; Thomas Bouet Guldbæk Poulsen[1]; Christopher Aboo[1]; Mikkel Eggert Thomsen[1]; Verena Tellstroem[2]; Dres Damgaard[3]; Claus Henrik Nielsen[3]; *[1]Aalborg University, Aalborg, Denmark; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Copenhagen University Hospital, Copenhagen, Denmark*

TP 461 **Quantitative analysis of in vivo methionine oxidation by heavy isotope labelling**; John Q Bettinger[1]; Kevin A Welle[1]; Jennifer R Hryhorenko[1]; Sina Ghaemmaghami[1]; *[1]University of Rochester, Rochester, NY*

PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS
TP 462-483

TP 462 **Optimizing enrichment of lowly abundant cellular retinol binding protein, type 1 (CRBP1) extracted from in-gel digest**; Stephanie M Zalesak[1]; Wenjing Li[1]; Jianshi Yu[1]; Maureen A Kane[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

TP 463   **Absolute quantitation of peptides by Coulometric Mass Spectrometry using ferrocene tags**; Praneeth Ivan Joel Fnu[1]; Hao Chen[1]; [1]*Department of Chemistry & Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102*

TP 464   **Protein digestion through superheating for fast mass spectrometry analysis of protein biomarkers**; Yuchen Wang[1]; Wenpeng Zhang[1, 2]; Zheng Ouyang[1]; [1]*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Department of Chemistry, Purdue University, West Lafayette, IN*

TP 465   **Development and Application of Extraction Methods for Quantification of Microcystins in Liver Tissue using LC-Orbitrap-MS**; David Baliu-Rodriguez[1]; Daria Kucheriavaia[1]; Dilrukshika S. W. Palagama[1]; Apurva Lad[1]; Grace M. O'neill[2]; Johnna A. Birbeck[2]; David J. Kennedy[1]; Steven T. Haller[1]; Judy A. Westrick[2]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH; [2]Wayne State University, Detroit, MI*

TP 466   **QPrEST+ validated isotope-labeled protein standard for absolute quantification using mass spectrometry**; Åsa Makower[1]; Marie Utterbäck[1]; Tove Boström[1]; Gabriella Jensen[1]; Laura Pozzi[1]; Sofié Olander[1]; Ulrika Qundos[1]; Björn Forsström[1]; [1]*Atlas Antibodies AB, Stockholm, Sweden*

TP 467   **Large Therapeutic Peptide Quantification in Human Plasma Using a Highly Sensitive and Robust Assay with HILIC to RP 2D-LC-MS/MS**; Moucun Yuan[1]; Meng Ye[2]; Yousef Basir[1]; Catherine Delguidice[1]; William R. Mylott[1]; Michael Cwik[2]; Mike Baratta[2]; [1]*PPD, Richmond, VA; [2]Takeda Pharmaceuticals International Co., Cambridge, MA*

TP 468   **Optimization of precursor and product ion m/z targets for tryptic peptide electrospray MS/MS analyses on triple quadrupole instruments**; Adrian R Woolfitt[1]; Maria I Solano[1]; Anne E Boyer[1]; John R Barr[1]; [1]*CDC, Atlanta, GA*

TP 469   **Highly sensitive quantitative analysis of Leuprolide from rat plasma using LC-MS/MS**; Ashutosh Shelar[1]; Purushottam Sutar[1]; Shailendra anil Rane[1]; Bhaumik Trivedi[1]; Shailesh Damale[1]; Anant Lohar[1]; Deepti Bhandarkar[1]; Navin Devadiga[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; [1]*Shimadzu Analytical (India) Pvt. Ltd, Mumbai, India*

TP 470   **New PRM-PASEF for highly multiplexed targeted acquisition in clinical samples**; Antoine Lesur[1]; Marta Mendes[1]; Jens Decker[2]; Sven Brehmer[3]; Schmit Pierre-Olivier[4]; Gunnar Dittmar[1]; [1]*Luxembourg Institute of Health, Strassen, Luxembourg; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Bruker Daltonique S.A., Wissembourg, France*

TP 472   **High Sensitive Detection and Qualitative Analysis of therapeutic peptides using MRM Analysis**; Faraz Rashid[1]; Dipankar Malakar[1]; Manoj Pillai[1]; [1]*SCIEX, 121,Udyog Vihar, Phase – IV, Gurgaon, Haryana, India*

TP 473   **Selective and sensitive quantification of glucagon in human plasma using microflow LC/Q-TOF MS**; Tomoya Kudo[1]; Wataru Fukui[1]; Toshiya Matsubara[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

TP 474   **Sample multiplexing with isotopic and isobaric TMT labeling for targeted pathway proteomics: application to aging mice**; Qing Yu[1]; Haopeng Xiao[2]; Mark P Jedrychowski[2]; Devin K Schweppe[1]; Jose Navarrete-Perrea[1]; Jeffrey Knott[3]; John C Rogers[4]; Edward T Chouchani[2]; Steven P Gygi[1]; [1]*Harvard Medical School, Boston, MA; [2]Dana-Farber Cancer Institute/ Harvard Medical School, Boston, MA; [3]Cell Signaling Technology, Danvers, MA; [4]Thermo Fisher Scientific, Rockford, IL*

TP 475   **Utilizing Differential Ion Mobility– Mass Spectrometry for Improved Immunopeptide Detection**; Elyssa Alvarez[1]; Tavleen K. Kochar[1]; James E. Keating[1]; Shengjie Chai[2]; Benjamin G. Vincent[3]; Sally A. Hunsucker[3]; Paul M. Armistead[3]; Gary L. Glish[1]; [1]*Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina; [2]Curriculum in Genetic & Molecular Biology, University of North Carolina, Chapel Hill, North Carolina; [3]Lineberger Comprehensive Cancer Center, University of North Carolina, Chapel Hill, North Carolina*

TP 476   **Quantitative analysis of Ras and AKT signaling pathways using a SureQuant targeted MS workflow**; Bhavin Patel[1]; Penny Jensen[1]; Aaron S Gajadhar[2]; Sebastien Gallien[3]; Andreas Huhmer[2]; Daniel Lopez-Ferrer[2]; Kay Opperman[1]; Ryan Bomgarden[1]; John C Rogers[1]; [1]*Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA*

TP 478   **Glycosylation improves stability of neuropeptides and elevates blood brain barrier (BBB) penetration**; Chenxi Liu[1]; Mitchell J. Bartlett[2]; Christopher R. Apostol[1]; Lajos Szabo[1]; Robin Polt[1]; Torsten Falk[2]; Michael L. Heien[3]; [1]*Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ; [2]Department of Neurology, The University of Arizona, Tucson, AZ; [3]Department of Chemistry and Biochemistry, University of Arizona, Tuscon, AZ*

TP 479   **A novel, simple and sensitive LC-MS/MS method for simultaneous quantification of insulin glargine and its metabolites (M1 and M2)**; Avinash B Gaikwad[1]; Atmakuri Chaitanya Krishna[1]; Yogesh Gorakhnath Arote[1]; Sujit Bhaskar Patil[1]; Jitendra Kelkar[2]; Ajit Datar[2]; Pratap Rasam[2]; [1]*Shimadzu Application Development Centre, Navi Mumbai, India; [2]Shimadzu Analytical (India) Pvt Ltd, Marol, Andheri, Mumbai, India*

TP 480   **Improving depth of coverage and absolute peptide detection limits using FAIMS separation coupled to a quadrupole-Orbitrap mass spectrometer**; Amirmansoor Hakimi[1]; Tabiwang N. Arrey[2]; Josh Nicklay[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Somerset, NJ*

TP 481   **Quantitation and Identification of Peptides by Free Radical Isobaric Tags for Relative and Absolute Quantitation**; Edgar M Manriquez[1]; Jinshan Gao[2]; *[1]Montclair State University, Montclair, NJ; [2]Montclair State University, Upper Montclair, NJ*

TP 482   **Influence of the N-terminal amino acid sequence on the expression of protein concatenating internal standard peptides for targeted proteomics**; Ayano Mori[1]; Tomohiro Kohata[1]; Ryotaro Yagi[1]; Yui Kaneko[1]; Takeshi Masuda[1]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto university, Kumamoto, Japan*

TP 483   **In Vitro Trileucine Stability Evaluation in Preclinical Species and Human Sera at 37 °C Using an LC-MS/MS Approach**; Ruipeng Mu[1]; Yue Huang[1]; Anton I Rosenbaum[1]; *[1]Clinical Pharmacology & Quantitative Pharmacology, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, South San Francisco, California*

PROCESS DEVELOPMENT MS
TP 484-489

TP 484   **Industry-wide Performance of the New Peak Detection Component of the Multi-Attribute Method**; Trina Mouchahoir[1, 2]; John Schiel[1, 2]; Rich Rogers[3]; *[1]National Institute of Standards and Technology, Gaithersburg, Maryland; [2]Institute for Bioscience and Biotechnology Research, Rockville, Maryland; [3]Bristol-Myers Squibb, Seattle, Washington*

TP 485   **Formulation differentiates the charge variants of a monoclonal antibody under thermal stresses**; Jun Zhang; *Amgen, Inc, Thousand Oaks, CA*

TP 486   **Highly Sensitive and Robust UPLC-MS/MS Quantification of Nitrosamine Impurities in Sartan and Ranitidine Drug Substances**; Mary E Lame[1]; Lindsay Hatch[2]; Dave Higton[3, 4]; Paul Rainville[1]; Gordon Fujimoto[2]; *[1]Waters Technologies Corporation, Milford, MA; [2]Waters Technologies Corporation, Beverly,, MA; [3]Waters Technologies Corporation, Wilmslow, United Kingdom; [4]Waters Technologies, Wilmslow, United Kingdom*

TP 487   **Making LC-MS Sensibly Useful for Host Cell Protein Applications**; Amy J Claydon[1]; St John Skilton[2]; A. Michelle English[3]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Protein Metrics, Inc., Cupertino, CA; [3]Protein Metrics Inc., Cupertino, CA*

TP 488   **Refinement of HR Multi-Attribute Method from Sample Preparation to Data Analysis**; Haichuan Liu[1]; Hao Yang[1]; Min Du[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 489   **Characterizing the Analytical Performance and Reliability of Spent Media Quantitation with an Integrated CE-MS Analyzer**; Kenion H Blakeman[1]; Ji Young L Anderson[1]; Colin M Gavin[1]; Kerin E Gregory[1]; Scott E Miller[1]; Glenn A Harris[1]; *[1]908 Devices, Inc., Boston, MA*

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY
TP 490-516

TP 490   **Hydroxyl-Radical Reaction Pathways for the Fast Photochemical Oxidation of Proteins Platform As Revealed by 18O Isotopic Labeling**; Roger (xiaoran) Liu[1]; Mengru Mira Zhang[1]; Bojie Zhang[1]; Don L. Rempel[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, st. louis, MO*

TP 491   **Ligand and Metal Binding to Wild Type and Mutant α-Synuclein**; Jaybree Lopez[1]; Carter Lantz[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

TP 492   **Structure and Effective Charge Characterization of Protein and protein complex in solution Using Mobility CE-MS**; Wenjing Zhang; *Beijing Institute of Techonology, Beijing, China*

TP 493   **Protein structural accessibility differences associated with Alzheimer's disease in cerebrospinal fluid by limited proteolysis-mass spectrometry**; Danielle A Faivre[1]; Eric L Huang[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

TP 494   **Fast Footprinting of proteins with Carbocations: The Hydrophobic Trifluomethoxy benzyl carbocation**; Jie Sun[1]; Xiaoran Liu[2]; Chunyang Guo[2]; Shuang Li[3]; Weikai Li[3]; Michael L. Gross[2]; *[1]Washington University in St.Louis, St.Louis, MO; [2]Washington University in St.Louis, St.Louis, Missouri; [3]Washington University School of Medicine, St. Louis, MO*

TP 495   **In-Depth Structural Analysis of G Protein-Coupled Receptors through Cross-Linking Mass Spectrometry**; Lisha Xia[1]; Ziliang Ma[1]; Jiahui Tong[1]; Yuliang Tang[2]; Wenqing Shui[1, 3]; *[1]ShanghaiTech University, Shanghai, China; [2]Peking University, College of Chemistry, Beijing, China; [3]iHuman Institute, ShanghaiTech University, Shanghai, China*

TP 496 **Delineating Metal-Mediated vs. Direct Protein Oxidation Pathways: Implications for Oxidative Modification Mapping in Metalloproteins**; Victor Yin[1]; Derek Holzscherer[1]; Lars Konermann[1]; [1]*University of Western Ontario, London, ON*

TP 497 **Characterization of an intrinsically disordered protein in its DNA-bound and unbound states using ultraviolet photodissociation and TIMS-MS**; Sarah N Sipe[1]; Kevin Jeanne Dit Fouque[2]; Alyssa Garabedian[2]; Fenfei Leng[2]; Francisco Fernandez-Lima[2]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*Florida International University, Miami, Florida*

TP 498 **Development of a multi-omics approach for the study of secondary envelopment in the beta herpesvirus Human Cytomegalovirus (HCMV)**; Hannah M. Britt[1]; Tristan Cragnolini[2]; Chris Hughes[3]; Johannes P.C. Vissers[3]; Konstantinos Thalassinos[1, 2]; [1]*University College London, London, United Kingdom;* [2]*Birkbeck College, University of London, London, United Kingdom;* [3]*Waters Corporation, Wilmslow, United Kingdom*

TP 499 **TMT-labeling assisted profiling of protein structure in human brain tissue of Alzheimer's disease**; Kaiwen Yu[1]; Mingming Niu[1]; Hong Wang[1]; Yuxin Li[1]; Zhiping Wu[1]; Junmin Peng[1]; [1]*St. Jude Children's research hospital, Memphis, TN*

TP 500 **Who's in charge: how metal ions define α-synuclein structure**; Rani Moons[1]; Albert Konijnenberg[1]; Anne-Marie Lambeir[1]; Frank Sobott[1, 2]; [1]*University of Antwerp, Antwerp, Belgium;* [2]*University of Leeds, Leeds, United Kingdom*

TP 501 **CCS measurements of lowly-charged (z < 3) electrosprayed proteins**; Ben Aguilar[1]; W Henry Benner[1]; [1]*Ion DX, Inc., Monterey, CA*

TP 502 **Investigating the Impact of Heparan Sulfate Domain Structure on Interleukin 8 Heparan Sulfate interactions**; Robert V Williams[1]; Tanvir Ahmed[1]; Pradeep Chopra[1]; Lifeng Sun[2]; Geert-Jan Boons[3]; I. Jonathan Amster[1]; [1]*University of Georgia, Athens, GA;* [2]*Utrecht University, Utrecht, Netherlands;* [3]*Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

TP 503 **Mass Spectrometry-based Characterization of Protein Structural Disruption Under Mechanochemical Stress Conditions**; Jazmine Crain[1]; Balasubrahmanyam Addepalli[1]; James Mack[1]; [1]*University of Cincinnati, Cincinnati, OH*

TP 504 **Measurement of the Stability of Immunoglobulin G Two by Cyclic Ion Mobility Spectrometry**; Kyle Buckley[1]; Lucas W Henderson[1]; Edie M Sharon[1]; David E. Clemmer[1]; [1]*Indiana University, Bloomington, IN*

TP 505 **Post-translational Modifications and Their Effects on the Conformation and Function of Hsp90 in Embryonic Stem Cells**; Seth W Mcnutt[1]; Feixia Chu[1]; Daniel T Thornton[1]; Hieu Nguyen[1]; [1]*University of New Hampshire, Durham, NH*

TP 506 **Distinguishing conformational changes of protein complexes based on unfolding pathways using Ion Mobility Mass Spectrometry, Collision-Induced Unfolding, and Molecular Modeling**; Stacey Nash[1]; Tyler Marcinko[1]; Richard W Vachet[2]; [1]*University of Massachusetts Amherst, Amherst, MA;* [2]*University of Massachusetts at Amherst, Amherst, MA*

TP 507 **Native Mass Spectrometry, Election-Capture Dissociation and Ion Mobility Collision-Induced Unfolding for Characterization of Ternary Protein Complex**; Jong Hee Song[1]; Jing Yan[1]; Nicole D. Wagner[1]; Aaron Balog[2]; Jing Li[2]; Richard Huang[2]; John Newitt[2]; Mark Witmer[2]; Louis Lombardo[2]; Olafur Gudmundsson[2]; Guodong Chen[2]; Gross L. Michael[1]; [1]*Washington University, St. Louis, MO;* [2]*Bristol-Myers Squibb Company, Princeton, NJ*

TP 508 **Domain orientation of the HS-binding protein Robo1 studied by IM-MS, NMR, and SAXS**; Robert Williams[1]; Jeong Y Yang[2]; Yunyun Gao[3]; Arwen Pearson[3]; Kelley Moremen[2]; James Prestegard[2]; Jon Amster[1]; [1]*University of Georgia, Athens, GA;* [2]*Complex Carbohydrate Research Center, University of Georgia, Athens, GA;* [3]*University of Hamburg, Hamburg, Germany*

TP 509 **Characterization of Common Human Histones using nESI-CIA-TIMS-MS**; Yasir Mamun[1]; Khoa Ngoc Pham[1]; Francisco A. Fernandez-Lima[1]; [1]*Florida International University, Miami, FL*

TP 510 **Conformational Analysis of Mtr4 using Hydrogen-Deuterium Exchange**; Naifu Zhang[1]; Keith J Olsen[2]; Sean J Johnson[2]; Sheena D'arcy[3]; [1]*UT Dallas, Richardson, TX;* [2]*Utah State University, Logan, UT;* [3]*UT Dallas, Richardson*

TP 511 **Structure-based validation can drastically under-estimate error rate in proteome-wide cross-linking mass spectrometry**; Haiyuan Yu[1]; Yugandhar Kumar[1]; Ting-Yi Wang[1]; Elnur Elyar Shayhidin[1]; [1]*Cornell University, Ithaca, NY*

TP 512 **Evidence in glioma that Ghost proteins are functional Regulators using large scale crosslink mass spectrometry and TurboID**; Tristan Cardon[1]; Etienne Coyaud[1]; Estelle Laurent[1]; Julien Franck[1]; Michel Salzet[1]; Isabelle Fournier[1]; [1]*PRISM, InsermU1192, Villeneuve d'ascq, France*

TP 513 **Modeling of a Sin3/HDAC Complex Sub-structure Using Crosslinking Mass Spectrometry (XL-MS)**; Charles A.S. Banks[1]; Yin Zhang[1]; Sayem Miah[1]; Yan Hao[1]; Mark K Adams[1]; Zhihui Wen[1]; Janet L Thornton[1]; Laurence Florens[1]; Michael P. Washburn[1]; [1]*Stowers Institute for Medical Research, Kansas City, MO*

TP 514   **Use of online buffer exchange coupled to native-mass spectrometry to elucidate the stoichiometry of the Salmonella FraR (transcriptional repressor)-DNA complex**; Angela Di Capua[1]; Blake E. Szkoda[1]; Venkat Golalpan[1]; Vicki H Wysocki[1]; [1]*The Ohio State University, Columbus, OH*

TP 515   **A conserved folding nucleus sculpts the complex free energy landscape of a highly divergent bacterial and archaeal TIM barrel enzyme**; Rohit Jain[1]; Khaja Muneeruddin[2]; Jeremy Anderson[3]; Michael J Harms[3]; Scott A Shaffer[2]; C. Robert Matthews[2]; [1]*Case Western Reserve University, Cleveland, OH;* [2]*University of Massachusetts Medical School, Worcester, MA;* [3]*University of Oregon, Eugene, OR*

TP 516   **Measuring protein conformational change in living cells by quantitative, comprehensive, and ultra-sensitive protein footprinting**; Jenna G. Caldwell[1]; Bjorn-Erik Wulff[1]; Lichao Zhang[2]; Joshua E. Elias[2]; Pehr A. B. Harbury[1]; [1]*Biochemistry, Stanford University School of Medicine, Stanford, CA;* [2]*Chan Zuckerberg BioHub, Stanford, CA*

PROTEOMICS: CLINICAL APPLICATIONS I
TP 517-535

TP 517   **The Prostate Cancer in vivo Secretome**; Amanda Khoo[1]; Joseph J. Otto[2]; Andrew Maclin[3]; Zhuyu Qui[4]; Vladimir Ignatchenko[3]; Katharina Fritsch[1]; Lydia Y. Liu[1]; Meinusha Govindarajan[1]; Danny Vesprini[5]; Julius O. Nyalwidhe[2]; Stanley Liu[5]; O. John Semmes[2]; Paul C. Boutros[4]; Thomas Kislinger[3]; [1]*University of Toronto, Toronto, ON;* [2]*Eastern Virginia Medical School, Norfolk, VA;* [3]*Princess Margaret Cancer Centre, Toronto, ON;* [4]*Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA;* [5]*Sunnybrook Health Sciences Centre, Toronto, ON*

TP 519   **Leukocyte proteomic profiling in first-episode schizophrenia patients: does oxidative stress play central roles in the pathophysiology network of schizophrenia**; Chao Peng[1]; Jie Jiang[2]; Chunling Wan[2]; [1]*National Facility for Protein Science, Zhangjiang Lab,SARI, CAS, Shanghai, 201210, China, shanghai, China;* [2]*Shanghai Jiao Tong University, Shanghai, China*

TP 520   **Development and Application of a Robust Methodology for In-Depth, Global and Phosphoproteome Measurements in Clinical Adipose Tissue**; James A Sanford[1]; Maria F Pino[2]; Marina A Gritsenko[1]; Chelsea M Hutchinson[1]; Joshua R Hansen[1]; Ronald J. Moore[1]; Wei-Jun Qian[1]; Lauren M Sparks[2]; Joshua N Adkins[1]; Paul Piehowski[1]; [1]*Pacific Northwest National Lab, Richland, WA;* [2]*AdventHealth, Orlando, FL*

TP 521   **PQ500 and SureQuant enables highly reproducible absolute quantification of 500 plasma proteins for clinical studies**; Jan Muntel[1]; Tejas Gandhi[1]; Huili Zhai[2]; Diana Shpektor[2]; David Yowe[2]; Jasison Jacob[2]; William Chutkow[2]; Karen Wang[2]; Sebastian Müller[1]; Yuehan Feng[1]; Roland Bruderer[1]; Lukas Reiter[1]; [1]*Biognosys, Schlieren, Switzerland;* [2]*Novartis Institutes for Biomedical Research, Cambridge, Massachusetts*

TP 523   **A Non-Hazardous "Green" Protocol for Proteomics of FFPE Tissues to Study the Progression of Breast Ductal Carcinoma by Label-Free Quantitation**; Georgia Mitsa[1, 2]; Christophe Goncalves[3]; Adriana Aguilar-Mahecha[3]; Qianyu Guo[1, 3]; Mark Basik[1, 4]; Alan Spatz[5]; Gerald Batist[1, 3, 6]; Wilson H. Miller, Jr. [1, 3, 7]; Sonia V. Del Rincon[1, 3]; René Zahedi[2]; Christoph H. Borchers[2, 3, 8]; [1]*Division of Experimental Medicine, McGill University, Montreal, QC;* [2]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [3]*Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC;* [4]*Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC;* [5]*Department of Pathology, Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [6]*Exactis Innovation, Montreal, QC;* [7]*Rossy Cancer Network, McGill University, Montreal, QC;* [8]*Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

TP 524   **Proteomic profiling of glycated serum proteins**; Yahor Vazmitsel[1]; Shawn Connolly[1]; Kuanysh Kabytaev[1]; [1]*University of Missouri, Columbia, MO*

TP 525   **Clinical application of multiple reaction monitoring-mass spectrometry (MRM-MS) to HER2 quantitation as potential diagnostics for breast cancer targeted therapy**; Misol Do[1]; Hyunsoo Kim[2]; Injoon Yeo[2]; Jihyeon Lee[1]; In Ae Park[3]; Han Suk Ryu[3]; Youngsoo Kim[1, 2]; [1]*Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea;* [2]*Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, South Korea;* [3]*Department of Pathology, Seoul National University College of Medicine, Seoul, South Korea*

TP 526   **Proteomics Analysis of Protein Profile Changes in Urine of Patients Suffering from Hashimoto´s Disease**; Tanja Panic-Jankovic[1]; Sandra Gaisbauer[2]; Goran Mitulovic[1]; [1]*Medical University of Vienna, KILM, Vienna, Austria;* [2]*Clinical Institute of Laboratory Medicine, Vienna General Hospital, Vienna, Austria*

TP 527   **Next generation potential biomarker candidates for Plasmodium vivax: Alternative to existing RDT?**; Shalini Aggarwal[1]; Apoorva Venkatesh[1]; Jayanthi Shastri[2]; Swati Patankar[1]; Sanjeeva Srivastava[3]; [1]*Indian Institute of Technology, Bombay, Mumbai, India;* [2]*T N Medical College & Nair Hospital, Mumbai, India;* [3]*IIT Bombay, Mumbai, India*

TP 528   **Discovery of blood biomarker for major mental illness by high-throughput plasma proteome profiling**; Hyeyoon Kim[1, 2]; Hyunsuk Shin[2]; Junghun Lee[2]; Dohyun Han[2, 3]; [1]*Department of Pathology, Seoul National University College of Medicine, Seoul, South Korea;* [2]*Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea;* [3]*Seoul National University Hospital, Seoul, South Korea*

TP 529   **In-depth serum profiling revealing novel protein biomarkers associated with Bechet disease diagnosis and therapy**; Linlin Cheng[1, 2]; Dongxue Wang[2]; Guibin Wang[2]; Ziyan Wu[3]; Meng Xu[2]; Xiaomei Zhang[2]; Liubing Li[1]; Chenxi Liu[1]; Jiayu Dai[2]; Songxin Yan[1]; Fuchu He[2]; Fengchun Zhang[3]; Xiaobo Yu[2]; Yongzhe Li[1]; [1]*Peking Union Medical College Hospital, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing, China;* [2]*State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences, Beijing Institute of Lifeomics, Beijing, China;* [3]*Peking Union Medical College Hospital, Peking Union Medical College and Chinese Academy of Medical Sciences, Key Laboratory of Rheumatology and Clinical Immunology, Beijing, China*

TP 530   **Multi-stage analysis of high-resolution mass spectrometry data reveals novel antimicrobial peptides (AMPs) in the cerebrospinal fluid of Alzheimer patients**; Satya Saxena[1]; Abhay Moghekar[2]; David R Goodlett[1, 3]; [1]*University of Maryland School of Dentistry, Baltimore, MD;* [2]*Department of Neurology, Hopkins University School of Medicine, Baltimore, MD;* [3]*University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland*

TP 531   **Proteomic Analysis of Exosomes Secreted During Epithelial to Mesenchymal Transition in Ovarian Cancer**; Carolina Thome[1, 2]; Germano Ferreira[1, 2]; Guilherme Lanfredi[2]; Francisco CJ Reis[2]; Marcus Smolka[3]; Vitor Faca[1, 2]; [1]*Center for Cell Based Therapy - University of Sao Paulo, Ribeirao Preto, Brazil;* [2]*Ribeirao Preto Medical School - University of Sao Paulo, Ribeirao Preto, Brazil;* [3]*Weill Institute for Cell and Molecular Biology - Cornell University, Ithaca, NY*

TP 532   **Simplified Sample Preparation Strategy for Plasma Proteomics and its Application to a Pilot Study of Ischemic and Non-Ischemic Cardiomyopathy Patients**; Meghan J. Mcfadden[1, 2]; Esha Joshi[3]; Douglas S. Lee[1, 4, 5]; Patrick R. Lawler[5]; Heather Ross[1, 5]; Filio Billia[1, 5, 6]; Anthony O. Gramolini[1, 6]; [1]*Ted Rogers Centre for Heart Research, Toronto, ON;* [2]*Institute of Biomaterials and Biomedical Engineering, University of Toronto, Toronto, ON;* [3]*Department of Molecular Genetics, University of Toronto, Toronto, ON;* [4]*ICES, University of Toronto, Toronto, ON;* [5]*Peter Munk Cardiac Centre, University Health Network, Toronto, ON;* [6]*Department of Physiology, University of Toronto, Toronto, ON*

TP 533   **A multi-omic surfaceome study identifies DLK1 as an epigenetically regulated protein and immunotherapeutic target in neuroblastoma**; Amber K. Weiner[1, 2]; Alexander B. Radaoui[2]; Matthew Tsang[2]; Dan Martinez[3]; Simone Sidoli; Karina L. Conkrite[2]; Alberto Delaidelli[4]; Jo Lynne Rokita[2]; Maria V. Lane[2]; Zalman Vaksman[2]; Komal S. Rathi[2]; Pichai Raman[2]; Jennifer Pogoriler[2]; Tricia Bhatti[2]; Bruce Pawel[5]; Beverly Teicher[6]; Stephen W. Erickson[7]; Poul H. Sorensen[4]; Yael P. Mosse[2, 8]; Kateryna Krytska[2]; Francesca Zammarchi[9]; Patrick H. Van Berkel[9]; Malcolm A. Smith[6]; Benjamin A. Garcia[1]; John M. Maris[2, 8]; Sharon J. Diskin[2, 8]; [1]*Department of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA;* [2]*Children's Hospital of Philadelphia, Philadelphia, PA;* [3]*Albert Einstein College of Medicine, Bronx, NY;* [4]*British Columbia Cancer Agency, Vancouver, BC;* [5]*Keck School of Medicine of USC, Los Angeles, CA;* [6]*National Cancer Institute, Bethesda, MD;* [7]*RTI International, Research Triangle Park, NC;* [8]*University of Pennsylvania, Philadelphia, PA;* [9]*ADC Therapeutics (UK) Ltd, London, United Kingdom*

TP 534   **In depth proteomics of the kidneys from autoimmune type I diabetes rat model through MALDI - Imaging Mass Spectrometry**; Konomi Uchida[1]; Yume Mukasa[1]; Kazuhiko Ishibashi[2]; Yuki Kuzuhara[1]; Takashi Nirasawa[3]; Ryo Kajita[3]; Hiroki Yanagi[3]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; [1]*Doshisha university, Faculty of Life and Medical Sciences, Kyoto, Japan;* [2]*ONO Pharmaceutical Co., Ltd., Fukui, Japan;* [3]*Bruker Japan K.K., Yokohama, Japan*

TP 535   **A multiplex targeted Mass spectrometry approach for the quantification of synuclein proteoforms in human biological fluids**; Marie-Laure Pons[1, 2]; Jerome Vialaret[1]; Stephane Moreau[2]; Sylvain Lehmann[1]; Christophe Hirtz[1]; [1]*IRMB, Univ Montpellier, INSERM, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France;* [2]*Shimadzu Europa GmbH, Duisburg, Germany*

PROTEOMICS: NEW APPROACHES II
TP 536-556

TP 536   **A combined proteomic and proteogenomic strategy helps decipher the zebrafish proteome**; Charlotte Macron[1]; Matthieu Porchet[1]; James Holzwarth[2]; Joy Richard[3]; Giulia Lizzo[3]; Philipp Gut[3]; Loïc Dayon[1, 4]; [1]*Proteomics, Nestlé Institute for Food Safety & Analytical Sciences, Nestlé Research, Lausanne, Switzerland;* [2]*Genomics, Nestlé Institute for Food Safety & Analytical Sciences, Nestlé Research, Lausanne, Switzerland;* [3]*Cell Biology, Nestlé Institute of Health Sciences, Nestlé Research, Lausanne, Switzerland;* [4]*Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland*

TP 537   **Multiproteomic approaches to study the epithelial-to-mesenchymal transition**; Paola Cavaliere[1]; Noah E. Dephoure[1]; [1]*Weill Cornell Medical College, New York, NY*

TP 538   **Proteome-wide detection of drug-target engagement with chaperone-dependent protein destabilization and degradation**; Taylur Ma[1]; Kelvin F Cho[2]; Christopher Rose[1]; Donald Kirkpatrick[1]; Robert Blake[1]; Kebing Yu[1]; *[1]Genentech Inc., South San Francisco, CA; [2]UC Berkeley, Berkeley, CA*

TP 539   **Deep nanogram-scale proteome profiling by isobaric labeling, extensive liquid chromatography, and mass spectrometry**; Danting Liu[1]; Jeffrey M. Sifford[1]; Zhiping Wu[1]; Boer Xie[1]; Kanisha Kavdia[1]; Kaiwen Yu[1]; Shu Yang[1]; Junmin Peng[1]; *[1]St jude Children's research hospital, Memphis, TN*

TP 540   **Comparison of Proteomic Analysis of Exosomes Purified Using Traditional Ultracentrifugation vs. Dialysis Concentration and Electropurification**; Elizabeth R Nunn[1]; James Wareham[1]; James N. Higginbotham[2]; Jeffrey Franklin[2]; Dennis K. Jeppesen[2]; Victor Pramov[3]; Siddarth Pratap[3]; Robert J Coffey[2]; Amy-Joan L. Ham[1]; *[1]Belmont University, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN; [3]Meharry Medical College, Nashville, TN*

TP 541   **Electron Transfer Dissociation Technique for Human Serum Albumin Adductomics**; Stanislau Stanisheuski[1]; Monica L V Maier[1, 2]; Yury Vasilev[1, 2]; David Williams[1, 2]; Dr. Claudia Susanne Maier[1, 2]; *[1]Oregon State Univeristy, Covallis, Oregon; [2]Linus Pauling Institute, Corvallis, Oregon*

TP 542   **Optimization of 16-plex Tandem Mass Tag Mass Spectrometry for large-scale proteomics**; Zhen Wang[1]; Kaiwen Yu[1]; Haiyan Tan[1]; Zhiping Wu[1]; Ji-Hoon Cho[1]; Xian Han[1, 2]; Thomas G. Beach[3]; Junmin Peng[1]; *[1]St jude Children's research hospital, Memphis, TN 38105; [2]University of Tennessee Health Science Center, Memphis, TN 38163; [3]Banner Sun Health Research Institute, Sun City, AZ 85351*

TP 543   **Integration of Nucleic Acid Extraction from Tissue Samples Into Standard Mass Spectrometry-Based Proteomic Workflows for Multi-'Omic Analysis of Clinical Samples**; Sandra E. Spencer Miko[1]; Ryan Riley[1]; Grace Cheng[1]; Karina Neilsen[1]; Gian Luca Negri[1]; Aaron H. Gillmor[2]; Ted Verhey[2]; Sorana Morrissy[2]; Gregg B. Morin[1, 2]; *[1]Canada's Michael Smith Genome Sciences Centre, Vancouver, BC; [2]University of Calgary, Calgary, AB*

TP 544   **Improving Proximity-labeling Proteomics Approach to Study Protein-protein Interactions**; Ashley M. Frankenfield[1]; Ling Hao[1]; *[1]George Washington University, Washington, DC*

TP 545   **A Method of High-Purity Extracellular Vesicle Enrichment from Microliter-scale Human Serum for Proteomic Analysis**; Xiaohui Ji[1, 2]; Sisi Huang[3]; Jie Zhang[1]; Zhijing Tan[1]; Yu Lin[1]; R. Kenneth Marcus[3]; Jianhui Zhu[1]; David M Lubman[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]Chongqing University Cancer Hospital, Chongqing, China; [3]Clemson University, Clemson, SC*

TP 546   **Two Dimensional Mass Spectrometry (2DMS): How Far Can We Go in Proteomics?**; Yuko Pui Yiu Lam[1]; Christopher A. Wootton[1]; Tomos E. Morgan[1]; Bryan P. Marzullo[1]; Cookson K. C. Chiu[1]; Alina Theisen[1]; Remy Gavard[1]; Meng Li[1]; Mark P. Barrow[1]; Peter B O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom*

TP 547   **Integrating Native IM-MS, Intact HRMS, and Bottom-Up Proteomics from Single Event Surface Sampling using Liquid Microextraction-nESI**; Raul Villacob[1]; Luke Richardson[1]; Fabrizio Donnarumma[2]; Kermit K Murray[2]; Touradj Kermit[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LOUISIANA*

TP 548   **Analysis of Metalloproteins in Pseudomonas aeruginosa Using Online Comprehensive Two-dimensional Active Modulation Liquid Chromatography**; Matthew Mcilvin[1]; Mak Saito[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA*

TP 549   **Exploring serum proteomes of 39 diverse mammal species: enabling comparative proteomics on a grand scale**; Benjamin A. Neely[1]; Magnus Palmblad[2]; Phillip A. Wilmarth[3]; Alison M. Bland[4, 5]; Michael G. Janech[4, 5]; *[1]National Institute of Standards and Technology, Charleston, SC; [2]Leiden University Medical Center, Leiden, Netherlands; [3]Oregon Health & Science University, Portland, Oregon; [4]College of Charleston, Charleston, SC; [5]Hollings Marine Laboratory, Charleston, SC*

TP 550   **Proteolytic resistant streptavidin increases dynamic range in affinity purification mass spectrometry workflows**; Jessica Read[1]; Ansgar Brock[1]; Jan Grunewald[1]; Shima Rayatpisheh[1]; John Venable[1]; Ajay Vashisht[1]; *[1]Genomics Institute of the Novartis Research Institute, San Diego, CA*

TP 551   **Multiplexed Analytical Platform using Affinity Capture and MALDI MS Enables Novel Assay Development for Screening Biomarkers of Neurological Diseases**; Vladislav B. Bergo[1]; Ghaith Hamza[2, 3]; Sergei Dikler[4]; Abhay Moghekar[5]; Sergey Mamaev[1]; Manor Askenazi[6]; Don M. Wojchowski[3]; Camilla Worsfold[1]; Jeffrey C. Silva[1]; *[1]ADEPTRIX CORP., Beverly, MA; [2]AstraZeneca, BioPharmaceuticals R&D, Discovery Sciences, Boston, MA; [3]University of New Hampshire, Durham, NH; [4]Bruker Scientific LLC, Billerica, MA; [5]Johns Hopkins University School of Medicine, Baltimore, MD; [6]Biomedical Hosting LLC, Arlington, MA 02474*

TP 552   **Transmembrane Electrophoresis Purification of Extracellular Vesicles using a Synthetic Peptide with Heat Shock Protein Affinity for Mass Spectrometry Analysis**; Philip Jakubec; *Dalhousie University, Halifax, NS*

TP 553   **SICyLIA-TMT: a multi-step labelling strategy for global redox proteomics**; Sergio Lilla[1]; Samuel Atkinson[1]; Jiska Van Der Reest[1]; Lisa Neilson[1]; Sara Rossana Zanivan[1]; *[1]The Beatson Institute for Cancer Research, Glasgow, United Kingdom*

TP 554 **A Proline- and Alanine-specific protease is complementary to trypsin in proteomics applications**; Diana Samodova[1]; Chris Hosfield[2]; Christian Necip Cramer[3]; Maria Valeria Giuli[4]; Giulia Franciosa[1]; Enrico Cappellini[5]; Michael Rosenblatt[2]; Christian Dahl Kelstrup[3]; Jesper Velgaard Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; [2]Promega Corporation, Madison, WI; [3]Novo Nordisk A/S, Måløv, Denmark; [4]University of Rome, Rome, Italy; [5]Natural History Museum of Denmark, University of Copenhagen, Copenhagen, Denmark*

TP 555 **Selective, sensitive and comprehensive detection of immune complex antigens for discovering disease-specific antigens**; Nozomi Aibara[1]; Mikirou Nakashima[1]; Naotaka Kuroda[1]; Kaname Ohyama[1]; *[1]Nagasaki University, Nagasaki, Japan*

TP 556 **Sample Preparation by Easy Extraction and Digestion (SPEED) - A Universal, Rapid, and Detergent-free Protocol for Proteomics**; Joerg Doellinger[1]; Andy Schneider[1]; Marcel Hoeller[1]; Peter Lasch[1]; *[1]Robert Koch-Institute, Centre for Biological Threats and Special Pathogens, Proteomics and Spectroscopy (ZBS6), Berlin, Germany*

> **PROTEOMICS: QUANTITATIVE I**
> **TP 557-573**

TP 557   **Systematic evaluation of protein synthesis inhibition through global quantification of newly synthesized proteins**; Ming Tong[1]; Suttipong Suttapitugsakul[1]; Senhan Xu[1]; Ronghu Wu[1]; [1]*Georgia Tech, Atlanta, GA*

TP 558   **In-depth proteome coverage and stoichiometric quantification of thiol-based redox modifications in mammalian tissues**; Tong Zhang[1]; Matthew J. Gaffrey[1]; Karl K. Weitz[1]; Ronald J. Moore[1]; Wei-Jun Qian[1]; [1]*Pacific Northwest National Lab, Richland, WA*

TP 559   **Label-free quantitative method for proteomics using one top peak intensity of peptides**; Ki Na Yun[1, 2]; Heeyoun Hwang[1]; Geul Bang[1]; Gun Wook Park[1]; Hye-Jung Kim[3]; Eugene Lee[4]; Yong-In Kim[4]; Jeong Hee Moon[5]; Sungho Yun[1]; Jong Shin Yoo[1]; Jin Young Kim[1]; [1]*Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; [2]Department of Chemistry, Sogang University, Seoul, South Korea; [3]K-bio health, Osong, South Korea; [4]Korea Research Institute of Standards and Science (KRISS), Daejeon, South Korea; [5]Disease Target Structure Research Center, KRIBB, Daejeon, South Korea*

TP 560   **A Comprehensive Evaluation of Variabilities Arising from Experimental Factors on LC-MS-based Proteomics Biomarker Discovery**; Min Ma[1, 2]; Shichen Shen[1, 3]; Shihan Huo[1]; Ming Zhang[1, 3]; Jun Qu[1, 3]; [1]*University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Institute, Buffalo, NY; [3]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

TP 561   **Effects to the human proteome due to legacy chemical exposure in the Great Lakes**; Emmalyn Dupree[1]; Bernard Crimmins[1]; Thomas Holsen[1]; James Pagano[2]; Brooke Thompson[3]; Krista Christensen[3]; Michelle Raymond[3]; Jonathan Meiman[3]; Costel C. Darie[1]; [1]*Clarkson University, Potsdam, NY; [2]SUNY Oswego, Oswego, NY; [3]Wisconsin Department of Health Services, Madison, WI*

TP 562   **Presynaptic protein dysfunction in the initial stages of amyloid proteotoxicity**; Timothy Hark[1]; Nalini R Rao[1]; Jeffrey Savas[1]; [1]*Northwestern University, Chicago, IL*

TP 563   **Integrated transcriptome and LC-MS/MS proteome analysis of early responses to herbivory-related decadienal in the marine diatom Phaeodactylum tricornutum**; Shahima Islam[1]; Michelle Gadush[1]; Maria D. Person[1]; Mona C Mehdy[1]; [1]*University of Texas at Austin, Austin, TX*

TP 564   **Examining the effect of deflazacort and prednisolone on skeletal muscle using cultured human myotubes and SILAC strategy**; Shefa M Tawalbeh[1, 2]; Tchilabalo D Alayi[1]; Emily Canessa[1]; Mansi V Goswami[1]; Yetrib Hathout[1]; [1]*School of Pharmacy and Pharmaceutical Sciences, State University of New York at Binghamton, Johnson City, New York; [2]Biomedical Engineering Department, State University of New York at Binghamton, Binghamton, New York*

TP 565   **Enhancement on IonStar Using Off-line Fractionation to Increase Protein Quantitative Depth**; Sailee Rasam[1, 2]; Shichen Shen[2, 3]; Shuo Qian[2, 4]; Jun Qu[1, 2, 3, 4]; [1]*Department of Biochemistry, University at Buffalo, Buffalo, New York; [2]Center of Excellence in Bioinformatics and Life Sciences, Buffalo, New York; [3]Department of Pharmaceutical Sciences, University at Buffalo, Buffalo, New York; [4]Department of Cell Stress Biophysical Oncology, Roswell Park Comprehensive Cancer Center, Buffalo, NY*

TP 566   **Multiple Reaction Monitoring and QconCAT Protein Standards Enable Targeted Absolute Quantification of Lysosomal Proteins**; Peter Mosen[1]; Roman Sakson[2]; Robert Hardt[1]; Biswajit Moharana[1]; Edgar Kaade[1]; Thomas Ruppert[2]; Volkmar Gieselmann[1]; Dominic Winter[1]; [1]*Institute for Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany; [2]Centre for Molecular Biology of Heidelberg University, Heidelberg, Germany*

TP 567   **Disruption-Compensation (DisCo) Analysis of RNA Polymerase II Interactome in Phosphatase Mutant**; Katlyn H Burriss[1]; Whitney R Smith-Kinnaman[1]; Guihong Qi[1]; Amber L Mosley[1]; [1]*Indiana University School of Medicine, Indianapolis, IN*

TP 568   **Multiplexed quantitative proteomics analysis of Human Brain Organoids**; Anita Saraf[1]; Chongbei Zhao[1]; Michaela E. Sardiu[1]; Gaye Hattem[1]; Tari J Parmely[1]; Laurence Florens[1]; Michael P. Washburn[1, 2]; [1]*Stowers Institute for Medical Research, Kansas City, MO; [2]Department of Pathology and Laboratory Medicine, University of Kansas Medical Center,, Kansas City, KS*

TP 569   **Quantitative Proteomic and Phosphoproteomic Profiling of Myocardial Remodeling in a Porcine Model of Left Ventricular Stiffening Following Chronic Repetitive Pressure-Overload**; Sailee Rasam[1, 2]; Brian R. Weil[3, 4]; John M. Canty[4, 5]; Jun Qu[1, 2, 6]; [1]*Department of Biochemistry, State University of New York, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, NY; [3]Department of Physiology and Biophysics, Buffalo, NY; [4]Clinical and Translational Research Center, Buffalo, NY; [5]Department of Medicine Jacobs School of Medicine & Biomedical Sciences, Buffalo, NY; [6]Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY*

TP 570   **Differentially Activated Signaling Pathways in Lymphatic Anomalies Cells**; Jong Min Choi[1]; Feng Jin[1]; Antrix Jain[1]; Alexander B. Saltzman[1]; Anna Malovannaya[1]; Wa Du[1]; Thuy Phung[1]; Sung Yun Jung[1]; [1]*Baylor College of Medicine, Houston, TX*

TP 571   **Insights into the Anti-cancer Effect Triggered by Silver Nanoparticles in Cisplatin-resistant A549 Lung Cancer Cells using Quantitative Proteomics**; Tin Yan Wong[1]; Kin Leung Kwan[2]; Henry H. N. Lam[1]; [1]*Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Kowloon, China;* [2]*Division of Life Science and Center for Chinese Medicine, The Hong Kong University of Science and Technology, Kowloon, China*

TP 572   **Identification of novel lysosomal proteins by magnetic nanoparticle enrichment and multi cell line SILAC background correction**; Fatema Akter[1]; Srigayatri Ponnaiyan[1]; Bianca Kögler-Mohrbacher[2]; Florian Bleibaum[3]; Markus Damme[3]; Bernhard Y Renard[4]; Dominic Winter[1]; [1]*Institute for Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany;* [2]*Bioinformatics Unit (MF1), Robert Koch Institute, Berlin, Germany;* [3]*Institute for Biochemistry, University of Kiel, Kiel, Germany;* [4]*Hasso Plattner Institute, University of Potsdam, Potsdam, Germany*

TP 573   **Understanding Cell Competition using Mass Spectrometry**; Suniya Khatun[1]; Konstantinos Thalassinos[1]; [1]*University College London, London, United Kingdom*

SMALL MOLECULES: QUALITATIVE ANALYSIS I
TP 574-589

TP 574   **An anomalous low codeine result linked to poppy seed ingestion solved by HRMS data analysis**; Ana Celia Grenier[1]; Philliip Hackett[1]; Lawrence J. Andrade[1]; [1]*Dominion Diagnostics, North Kingstown, RI*

TP 575   **A product ion may conceal another! How very high-resolution may be necessary to undoubtly identify a therapeutic substance metabolite**; Annelaure Damont[1]; Vivian Delcourt[2]; Stéphane Trevisiol[2]; Yves Moulard[2]; Patrice Garcia[2]; Ludovic Bailly-Chouriberry[2]; Christophe Junot[1]; François Fenaille[1]; Jean-Claude Tabet[1, 3]; [1]*Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France;* [2]*GIE-LCH, Laboratoire des Courses Hippiques, Verrières-le-Buisson, France;* [3]*Sorbonne Universités, UPMC Univ Paris 06, CNRS, IPCM, Paris, France*

TP 576   **Identifying food and environmental contaminants using the new NIST High-Res MS/MS Library search algorithms and publicly available LC/MS/MS spectral libraries**; Emma E. Rennie[1]; Frank Kuhlmann[1]; James S. Pyke[1]; Stephen Madden[1]; O. David Sparkman[2]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*University of the Pacific, Stockton, CA*

TP 577   **An Efficient Approach to Oligomer Screening in Extractables from Single-Use Systems**; Emily Volk[1]; Bin Sun[1]; Rolf Kern[2]; Owen Perlowski[1]; Benben Song[1]; [1]*Pall Corporation, Westborough, MA;* [2]*SCIEX, Redwood Shores, California 1201*

TP 578   **ms.epfl.ch on-line tool, new functionalities**; Daniel Ortiz[1]; Natalia Gasilova[1]; Francisco Sepulveda[1]; Luc Patiny[1]; Laure Menin[1]; [1]*EPFL, Lausanne, Switzerland*

TP 579   **Quantification and Confirmation of Nitrosamine impurities in Active Pharmaceutical Ingredients (API) of Sartan Drugs Using MRM To MS/MS Detection**; Chandra Sekar[1]; Aman Sharma[1]; Sandeep Choudhary[1]; Manoj G Pillai[1]; [1]*Sciex, Gurugram, India*

TP 580   **Substituent Effects on the Fragmentation pathway of Anthraquinone Dyes from the Weaver Dye Library: A Tandem Mass Spectrometry approach**; Julio E Teran[1]; Yufei Chen[1]; Xinyi Sui[1]; Tim Stratton[2]; Nelson Vinueza[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*Thermo Fisher Scientific, Austin, TX*

TP 581   **HCN emission by a millipede detected remotely by reactive adsorption on Gold nanoparticles followed by laser desorption/ionization mass spectrometry (LDI-MS)**; Julius Pavlov[1]; Sihang Xu[1]; Kipling Will[2]; Brandt Weary[2]; Athula B. Attygalle[1]; [1]*Stevens Institute of Technology, Hoboken, NJ;* [2]*UC Berkeley, Berkeley, CA*

TP 582   **Monitoring Enzymatic Reactions by LC/Single Quad to Gain Insights on Reaction Mechanisms**; Kyle J Covert[1]; Carim Van Beek[2]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*University of the Pacific, Stockton, CA*

TP 584   **Integrated qualitative analysis of volatile compounds from beer by using SPME-GC-HRTOFMS with EI/FI**; Koji Okuda[1]; Michael C Long[2]; Lynda McMaster-Schuyler[3]; Jacob T Shelley[4]; A John Dane[1]; Robert B Cody[1]; [1]*JEOL USA, Inc., Peabody, MA;* [2]*Center for Biotechnology and Interdisciplinary Studies, Rensselaer Polytechnic Institute, Troy, NY;* [3]*Department of Natural Sciences and Math, SUNY Cobleskill, Cobleskill, NY;* [4]*Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Cogswell Laboratory, Troy, NY*

TP 585   **A fast screening approach based on SONAR acquisition and UNIFI library for hepatotoxic pyrrolizidine alkaloids from herbal medicines and preparations**; Fen Xiong[1]; Aizhen Xiong[1]; Yanchao Shi[2]; Ming Yuan[2]; Kate Yu[2]; Li Yang[1]; Zhengtao Wang[1]; [1]*Institute of Chinese Materia Medica, Shanghai University of Traditional Chinese Medicine, shanghai, China;* [2]*Waters Corporation Shanghai Science & Technology Co Ltd, shanghai, China*

TP 586   **A case study of the MassChemsite Reaction Tracking workflow: detecting and identifying byproducts during PROTAC synthesis**; Laura Goracci[1]; Elisabeth Ortega-Carrasco[2]; Ismael Zamora[2, 3]; Fabien Fontaine[2]; Jenny Desantis[1]; [1]*Department of Chemistry, Biology, and Biotechnology, University of Perugia, Perugia, Italy;*

[2]*Lead Molecular Design S.L., Sant Cugat de Valles, Spain;* [3]*Molecular Discovery, Ltd., Borehamwood, United Kingdom*

TP 587   **Unknown Constituent Identification in Topical Preparation using a Q-TOF Mass Spectrometer**; Evelyn H. Wang[1]; Helen Hao[1]; Jeffrey H. Dahl[1]; Jennifer C. Davis[1]; Priyanka Chitranshi[1]; Katie Pryor[1]; Christopher T. Gilles[1]; [1]*Shimadzu Scientific Instruments Inc., Columbia, MD*

TP 588   **Screening and Identification of extractables in drug container by high-resolution accurate mass LC-MS/MS operated in polarity switching mode**; Prasanth Joseph[1]; Saikat Banerjee[1]; Samir Vyas[2]; [1]*Agilent Technologies, BENGALURU, India;* [2]*Agilent Technologies, Mumbai, India*

TP 589   **A Simple, High-Throughput UHPLC-HRMSMS Method for Quantitation of Purine Metabolites in Tissue**; Taylor A. Harmon[1]; Daniela Salvemini[2]; Richard A Yost[1]; Timothy J Garrett[1]; [1]*University of Florida Department of Chemistry, Gainesville, FL;* [2]*St. Louis University Department of Physiology and Pharmacology, St. Louis, MO*

STABLE ISOTOPE LABELING
TP 590-602

TP 590   **Selective Pulse Chase-SILAC Labeling of Three-Dimensional Multicellular Spheroids for Global Proteome Analysis**; Nicole C. Beller[1]; Jessica K. Lukowski[2]; Amanda B. Hummon[1]; [1]*The Ohio State University, Columbus, OH;* [2]*University of Notre Dame, Notre Dame, IN*

TP 591   **Vascular beds proteome dynamics in vascular dysfunction induced by an acute inflammatory response**; Aida Serra[1]; Xavier Gallart-Palau[1, 2]; [1]*+Pec Proteomics, IMDEA Food Research Institute, Madrid, Spain;* [2]*IISPV, Hospital Universitari Institut Pere Mata, Reus, Spain*

TP 592   **TMTpro16plex Reagents Reach New Sample Multiplexing Heights at Proteome-scale Depths in Quantitative Proteomics**; Jiaming Li[1]; Jonathan Van Vranken[2]; Laura Pontano Vaites[1]; Devin Schweppe[1]; Edward L Huttlin[1]; Chris Etienne[3]; Premchendar Nandhikonda[3]; Rosa Viner[4]; Aaron M Robitaille[5]; Andrew Thompson[6]; Karsten Kuhn[6]; Ian Pike[6]; Ryan Bomgarden[3]; John Rogers[3]; Steven Gygi[1]; Joao A. Paulo[1]; [1]*Harvard Medical School, boston, MA;* [2]*Harvard Medical School, Boston, MA;* [3]*Thermo Fisher Scientific, Rockford, IL;* [4]*ThermoFisher Scientific, San Jose, CA;* [5]*Thermo Fisher Scientific, San Jose, CA;* [6]*Proteome Sciences, London, United Kingdom*

TP 593   **[1,2-13C2]-L-glutamine mass isotopomers map hepatic mitochondrial metabolism without tracer interference**; Stephan Siebel[1]; Rebecca L Cardone[1]; Abudukadier Abulizi[1]; Raaisa Raaisa[1]; Richard M Williams[1]; Raghav Sehgal[1]; Gina M Butrico[1]; Gary W Cline[1]; Douglas L Rothman[1]; Graeme F Mason[1]; Richard G Kibbey[1]; [1]*Yale University, New Haven*

TP 594   **21-plex Isobaric Multiplex Reagents for Carbonyl Containing Compounds (SUGAR) tags for high-throughput MS2-level glycan characterization and relative quantification**; Zicong Wang[1]; Miyang Li[2]; Yu Feng[1]; Lingjun Li[1, 2]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222*

TP 595   **Fructose Fluxomics of Fatty Acid Treated HepRG Cells to predict flux in NASH patients via LC-HRMS**; Kyle Wald[1]; Anitha Saravankumar[2]; Matthew Blatnik[1]; Fatemeh Akhlaghi[2]; [1]*Pfizer Inc., Groton, CT;* [2]*University of Rhode Island, South Kingstown, RI*

TP 596   **Optimization of LC-MS/MS conditions to improve the proteome coverage in 16-plex tandem mass tag-based proteomics**; Shu Yang[1]; Mingming Niu[1]; Zhen Wang[1]; Zhiping Wu[1]; Huan Sun[1]; Kaiwen Yu[1]; Danting Liu[1]; Junmin Peng[1]; [1]*St. Jude Children's Research Hospital, Memphis, TN 38105*

TP 597   **Detecting stable isotope labeled metabolites in untargeted analysis utilizing a benchtop Orbitrap mass spectrometer and a single processing software platform**; Amanda Souza[1]; Ioanna Ntai[1]; Tatjana Talamantes[1]; Ralf Tautenhahn[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

TP 598   **Resolution of 13C and Deuterium Isotopes Allows High-Sensitivity Lipid Fluxomics Analysis Gives Insight into Post-Prandial Lipid Metabolism**; Matthew Mitsche[1]; Xiaorong Fu[2]; Jeffrey Mcdonald[2]; [1]*UTSW, Dallas;* [2]*University of Texas Southwestern Medical Center, Dallas, TX*

TP 599   **Stable Isotope-Resolved Metabolomics characterization of FLCN-deficient renal cancer cells and tissues using Ultra-High-Resolution Mass Spectrometry**; Ye Yang[1]; Daniel R. Crooks[1]; Richard M. Higashi[2]; Teresa W.M. Fan[2]; Andrew N. Lane[2]; Laura S. Schmidt[1]; W. Marston Linehan[1]; [1]*National Institutes of Health, Bethesda, MD;* [2]*University of Kentucky, Lexington, KY*

TP 600   **HRMS/MS-Based Approach for Separation and Quantification of Stable Isotope-Labeled Marfey's Reagent Derivatized Physiological Amino Acids Stereoisomers**; Nitish R. Mishra[1]; Amar Deep Sharma[1]; William G. Gutheil[1]; [1]*University of Missouri-Kansas City, Kansas City, MO*

TP 601   **Measurement of trace amounts of carbon dioxide in water by MS - How hard can that be?**; Colton Breyer[1]; Aaron G. Nash[1]; Thomas Chi Cao[1]; Dale A. Chatfield[1]; Douglas B. Grotjahn[1]; Diane K. Smith[1]; [1]*Dept. Chemistry and Biochemistry, San Diego State University, San Diego, CA*

TP 602   **Studying the temporal dynamics of the gut microbiota using metabolic stable isotope labeling and metaproteomics**; <u>Patrick Smyth</u>[1]; Xu Zhang[1]; Zhibin Ning[1]; Janice Mayne[1]; Jasmin I Moore[1]; Krystal Walker[1]; Mathieu Lavallée-Adam[1]; Daniel Figeys[1]; *[1]University of Ottawa, Ottawa, ON*

ANTIBODIES & ANTIBODY DRUG CONJUGATES III
WP 001-015

WP 001 **The impact of mass spectrometry analysis on drug discovery of a human IgG2 bispecific antibody**; Jia Dong[1]; Bryant Chau[1]; Feng Wang[1]; Gavin Dollinger[1]; Pavel Strop[1]; Arvind Rajpal[1]; [1]*Bristol-Myers Squibb, Redwood City, CA*

WP 002 **A Three Dimensional Plug-And-Play Ultra Performance Liquid Chromatography and Native Mass Spectrometry System for the Analysis of Biotherapeutics**; Mengxuan Jia[1]; Olivier Jean-Baptiste Mozziconacci[1]; [1]*MRL Analytical Sciences, Merck & Co. Inc., Rahway, NJ*

WP 003 **Sensitive drug distribution measurements of an ADC with non-denaturing capillary SEC**; Guillaume Tremintin[1]; Yue Ju[1]; Pan Mao[2]; Melvin A. Park[3]; [1]*Bruker, San Jose, CA; [2]Newomics, Berkeley, CA; [3]Bruker Daltonics, Billerica, MA*

WP 004 **Mass Spectrometric Characterization of Antibody-siRNA Conjugate using the Agilent 6545XT AdvanceBio LC/Q-TOF**; David Wong[1]; Balu Palani[2]; [1]*Agilent Technologies, Inc., Santa Clara, CA; [2]Avidity Biosciences, Inc., La Jolla, CA*

WP 005 **Evaluating the Sensitivity of the Synapt XS Mass Spectrometer for Analysis of Intact Monoclonal Antibody**; Malcolm Anderson[1]; Lucy Fernandes[2]; Heidi Gastall[1]; Laetitia Denbigh[2]; Joanne Ballantyne[2]; Samantha Ippoliti[3]; [1]*WATERS, Cheshire, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corps, Milford, MA*

WP 006 **Comparative Analysis of Glycopeptides between Biologics and Biosimilar of Infliximab by LC-ESI-MS/MS**; Hyejin Kim[1, 2]; Geul Bang[1]; Myung Jin Oh[2]; Hyun Joo An[2]; Jin Young Kim[1]; Heeyoun Hwang[1]; Jong Shin Yoo[1, 2]; [1]*Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; [2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejoen, South Korea*

WP 007 **A novel peptide-based quantification strategy to identify biomarkers from LFQ-based quantitative-proteomics data**; Deeptarup Biswas[1]; Chetanya Gupta[1]; Sanjeeva Srivastava[2]; [1]*IIT Bombay, Mumbai, India; [2]IIT Bombay, Mumbai, India*

WP 008 **Mapping a Conformational Epitope of Hemagglutinin A Using Native MS and Ultraviolet Photodissociation**; M. Rachel Mehaffey[1]; Keith R. Morgenstern[1]; Jiwon Lee[1]; Jiwon Jung[1]; Michael B. Lanzillotti[1]; Edwin E. Escobar[1]; George Georgiou[1]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 009 **An Intact Protein MS and MAM Approach for In Vivo Monitoring of Bispecific Antibody Product Quality Attributes** ; John F. Kellie[1]; Nicole A. Schneck[1]; Matthew E. Szapacs[1]; [1]*GSK, Collegeville, PA*

WP 010 **Middle-down Antibody Characterization Using ExD-based Fragmentation in a Q-TOF**; Joseph C. Meeuwsen[1, 2]; Michael C. Hare[1]; Diana M. Oppenheimer[1]; Valery G. Voinov[1, 2]; Joseph S. Beckman[1, 2]; [1]*e-MSion, Inc., Corvallis, OR; [2]Oregon State University, Corvallis, OR*

WP 011 **A deep learning model for similarity evaluation between biologics and biosimilars using intact glycoproteins analysis by LC-Q-TOF MS**; Geul Bang[1, 2]; Hyejin Kim[3]; Myung Jin Oh[3]; Hyun Joo An[3]; Heeyoun Hwang[1]; [1]*Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; [2]College of Pharmacy, Korea University, Jochiwon, South Korea; [3]Graduate School of Analytical Science and Technology, Chungnam National University, Daejoen, South Korea*

WP 012 **A versatile method for quantitation of methionine oxidation in Fc fragment of therapeutic monoclonal antibodies using stabile-isotope labelled internal standards**; Tomasz K Gozdziewicz; *Polpharma Biologics, Gdansk, Poland*

WP 013 **Advancing mAb characterization with microchip CE-MS coupled to a PASEF enabled QTOF**; J. Scott Mellors[1]; Guillaume Trementin[2]; Scott B Ficarro[3, 4]; Jarrod A Marto[3, 4]; [1]*908 Devices, Inc., Carrboro, NC; [2]Bruker Scientific, San Jose, CA; [3]Departments of Cancer Biology and Oncology Pathology, Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA; [4]Department of Pathology, Brigham and Women's Hospital and Harvard Medical School, Boston, MA*

WP 014 **LCMS characterization of a mouse monoclonal antibody used as a ligand binding assay reagent**; Qing Xie[1]; Valerie Quarmby[2]; Jihong Yang[2]; [1]*Genentech, South SF, CA; [2]Genentech Inc, South San Francisco, CA*

WP 015 **Deep Identification and Relative Quantitation of Unknown HCPs in Antibody Using an Optimized Sample Preparation Combined with nanoLC-MS**; Sun Jianan[1]; Zhou Yue[2]; Bo Tao[1]; [1]*ThermoFisher, Beijing,China, China; [2]ThermoFisher Scientific, Shanghai, China*

ART, ARCHAEOLOGY & PALEONTOLOGY
WP 016-020

WP 016 **Mass Spectrometric Identification of Collagen Preserved in Paleolithic Animal Remains**; Takashi Nakazawa[1]; Momoko Osawa[2]; Mako Inuzuka[1]; Kazuki Kawahara[3]; Seiji Kadowaki[2]; Yoshihiro Nishiaki[4]; [1]*Nara Women's University, Nara, Japan;* [2]*Nagoya University, Nagoya, Japan;* [3]*Osaka University, Suita, Japan;* [4]*University of Tokyo, Bunkyo-ku, Japan*

WP 017 **Organic compounds in the textile bandage of the Egyptian mummy**; Olga Polyakova[1]; Viatcheslav Artaev[2]; Olga Vasilyeva[3]; Maria Mednikova[4]; Jenya Anokhina[3]; Albert T Lebedev[1]; [1]*Moscow State University, Moscow, Russian Federation;* [2]*Leco Corporation, St. Joseph, MI;* [3]*Pushkin Museum, Moscow, Russia;* [4]*Institute of archaeology RAS, Moscow, Russia*

WP 018 **Expansion of the moa bone proteome and post-translational modifications**; Elena Schroeter; *North Carolina State University, Raleigh, NC*

WP 019 **Collagen decay studies in aged bone for archaeological applications**; Kevin Anderson[1]; Brian Thomas[2]; Lucien Tuinstra[2]; Stephania Herodotou[2]; Peter Myers[2]; Stephen Taylor[2]; [1]*Arizona Christian University, Glendale, AZ 85306;* [2]*University Of Liverpool, Liverpool, United Kingdom*

WP 020 **Identification approaches of the efflorescence detected in Infinity of Nations at the Smithsonian National Museum of the American Indian**; Alba Alvarez-Martin[1]; John George[2]; Emily Kaplan[2]; Lauren Osmond[2]; Leah Bright[2]; G. Asher Newsome[1]; Gwénaëlle Kavich[1]; Rachel Kaczkowski[1]; Susan Heald[2]; [1]*Museum Conservation Institute, Smithsonian Institution, Suitland, MD;* [2]*The National Museum of the American Indian, Smithsonian Institution, Washington, DC*

BIG ION MS
WP 021-023

WP 021 **Characterization of macromolecular complexes using multistage ultraviolet photodissociation mass spectrometry**; Ines C Santos[1]; Jada N. Walker[1]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 023 **Superconducting Tunnel Junction Cryodetection Analysis of Bacteriophage Qbeta Capsid by MALDI TOF MS and ESI LIT MS**; Li-Xue Jiang[1]; Liam Dugan[1]; Arezoo Shahrivarkevishahi[2]; Jeremiah J. Gassensmith[2]; Mark E. Bier[1]; [1]*Carnegie Mellon University, Pittsburgh, PA;* [2]*University of Texas at Dallas, Richardson, TX*

BIOMARKERS: DISCOVERY II
WP 025-042

WP 025 **Quantitative Top-Down Proteomics of Human Tears Reveals Proteoform Changes Related to Age**; Mick Greer[1]; Daniel Lopez-Ferrer[2]; Romain Huguet[2]; Peter Verhaert[3]; Greg Foster[4]; Vlad Zabrouskov[2]; Andreas Huhmer[2]; Peter Raus[5]; Ken Durbin[6]; Joe Greer[6]; Ryan Fellers[6]; Rich Leduc[6]; [1]*Thermo Fisher Scientific, Austin, TX;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*ProteoFormiX, Beerse, Belgium;* [4]*ThermoFisher Scientific, South San Francisco, CA;* [5]*Vrije Universiteit Brussel, Brussels, Belgium;* [6]*Proteinaceous, Evanston, IL*

WP 026 **DNA Aptamer Epitope Analysis as Antibody Alternatives Opens New Approaches for Biomarker Elucidation and Molecular Diagnostics**; Michael Przybylski[1]; Loredana Lupu[1]; Pascal Wiegand[1]; Nico Huettmann[1, 2]; Stephan Rawer[1]; Wolfgang Kleinekofort[1, 3]; Alexander Lazarev[4]; Maxim Berezovski[2]; [1]*Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spec, Ruesselsheim, Germany;* [2]*University of Ottawa, Ottawa, ON;* [3]*Rhein Main University, Ruesselsheim, Germany;* [4]*Pressure Biosciences Inc., South Easton, MA*

WP 027 **Detailed characterization of aged human brain gangliosidome by high resolution multistage mass spectrometry**; Raluca Ica[1]; Alina Petrut[2]; Mirela Sarbu[2]; Zeljka Vukelić[3]; Alina D. Zamfir[2]; [1]*National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania;* [2]*National Institute for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania, TIMISOARA, Romania;* [3]*Department of Chemistry and Biochemistry, University of Zagreb Medical School, Zagreb, Croatia, Zagreb, Croatia*

WP 028 **Glycopeptide Biomarkers in Serum Haptoglobin for Hepatocellular Carcinoma Detection in Patients with Non-Alcoholic Steatohepatitis**; Jianhui Zhu[1]; Junfeng Huang[2]; Jie Zhang[1]; Zhengwei Chen[2]; Yu Lin[1]; Gabriela Grigorean[1]; Lingjun Li[2]; Suyu Liu[3]; Amit G. Singal[4]; Neehar D. Parikh[1]; David M. Lubman[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*University of Wisconsin-Madison, Madison, WI;* [3]*UT MD Anderson Cancer Center, Houston, TX;* [4]*University of Texas Southwestern Medical Center, Dallas, TX*

WP 029 **Combined NMR and LCMS metabolomics approach reveals candidate metabolite markers for whole body radiation exposure**; Kiran Maan[1]; Ruchi Baghel[2]; Radhika Bakhshi[3]; Poonam Rana[2]; [1]*Institute of Nuclear Medicine & Allied Sciences (INMAS) - DRDO, Delhi, India;* [2]*Institute of Nuclear Medicine & Allied Sciences (INMAS) - DRDO, Delhi, India;* [3]*Shaheed Rajguru College of Applied Sciences for Women (SRCASW), University of Delhi, Delhi, India*

WP 031 **MALDI-nanochip based Screening of Exosomal Biomarkers: Application to Cancer Diagnostics**; Michael Douglas Nairn[1]; Michael Wuczkowski[2]; Jesús Jiménez[3]; Iris Prinz[4]; Marco Rissoglio[5]; Emanuele Barborini[5, 6]; Gerald Stübiger[7]; [1]*Shimadzu, Manchester, UK, Manchester, United Kingdom;* [2]*Medical University of Vienna,*

Vienna, Austria; [3]Clover Bioanalytical Software, Granda, Spain; [4]Stratec Consumables,, Salzburg, Austria; [5]Tethis, Milan, Italy; [6]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; [7]Comprehensive Cancer Center, Vienna, Austria

WP 032 **Metabolite and Lipid Profiling in Human Serum Related to Rheumatoid Arthritis**; Yan-Ping Lin[1]; Weixuan Chen[2]; Rong Meng[1]; Gary W. Caldwell[1]; Wensheng Lang[1]; *[1]Janssen R&D LLC., Spring House, PA; [2]Janssen R&D LLC., San Diego, CA*

WP 033 **Large-Scale Site-Specific Glycopeptides Screening from Human Serum as Novel Biomarkers for Non-Alcoholic Steatohepatitis using Stepped HCD-MS/MS**; Yu Lin[1]; Jianhui Zhu[1]; Jie Zhang[1]; Zhijing Tan[1]; Lingyun Pan[1]; David M Lubman[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 034 **Comprehensive proteomic profiling of stool from IBD patients reveals biomarkers of disease activity**; Brandon Harder[1]; Annemarie N Lekkerkerker[1]; Ellen P Casavant[1]; Marco Prunotto[1]; Jacqueline M McBride[1]; W Rodney Mathews[1]; Veronica G Anania[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 035 **An Ultra High-throughput Plasma Protein Profiling (uHTPPP) Workflow Using a Modified Quadrupole-Orbitrap Mass Spectrometer**; Michelle Dubuke[1]; Sarah Trusiak[1]; Ryan D. Bomgarden[2]; Sergei Snovida[2]; Bhavin Patel[2]; Emily Chen[3]; *[1]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [2]Thermo Fisher Scientific, Rockford, IL; [3]Thermofisher Scientific Precision Medicine Science Center, Cambridge, MA*

WP 036 **Measurement of serum LPAs as potential biomarkers for COPD disease**; Qingling Li[1]; Wei Tew[1]; Andrew Birnberg[1]; Arindam Chakrabarti[1]; Erik Verschueren[1]; Carrie Rosenberger[1]; Michele Grimbaldeston[1]; Wendy Sandoval[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 039 **High-sensitivity Proteoform Profiling of Apolipoproteins A-I and A-II in 150 Individuals: Characterizing the Association of Proteoforms to Cardiometabolic Phenotype**; Henrique Dos Santos Seckler[1]; John T. Wilkins[2]; Jonathan Scott Rink[2]; Luca Fornelli[3]; Richard D Leduc[1]; Ryan T Fellers[1]; C Shad Thaxton[1]; Allan Sniderman[4]; Donald M lloyd-jones[2]; Philip D. Compton[5]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Chicago, IL; [3]University of Oklahoma, Norman, OK; [4]McGill University, Montreal, QC; [5]Integrated Protein Technologies, Inc., Evanston, IL*

WP 040 **Utilizing Erythrocytes as Sources of Biomarkers for Alzheimer's Disease**; Jericha Mill[1]; Vihar Patel[2]; Tyler Ulland[2]; M. S. Salamat[2]; Ozioma Okonkwo[3]; Thomas Raife[2]; Lingjun Li[1, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; [2]Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; [3]Clinical Science Center, Wisconsin Alzheimer's Disease Research Center, University of Wisconsin School of Medicine and Public Health, Madison, Wisconsin; [4]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

WP 041 **Integrative discovery approach to identification of biomarkers in Fabry disease patient biofluids**; Lisa A Crawford[1]; Maria Stella Ritorto[1]; *[1]Sanofi, Framingham, MA*

WP 042 **Global Analysis of Protein Folding Stability Changes in a Mouse Model of Parkinson's Disease**; Michael C. Fitzgerald[1]; Renze Ma[1]; Julia Johnson[1, 2]; *[1]Duke University, Durham, NC; [2]Washington University in St.Louis, St.Louis, Missouri*

BIOMARKERS: QUANTITATIVE ANALYSIS II
WP 043-061

WP 043 **Mass Spectrometry-Based Proteogenomics Analysis of Serum EGFR Family Proteins in Patients with Solid Tumors**; Yun Chen[1]; Yuanyuan Zhang[1]; *[1]Nanjing Medical University, Nanjing, China*

WP 044 **A Novel Derivatization Procedure for the Chemicals with Carboxylic Acid and Its Application in LC-MS/MS Bioanalysis**; Dawei Zhou[1]; Yajie Zhang[1]; Sharon Tong[1]; *[1]WuXi AppTec, Cranbury, NJ*

WP 045 **UPLC-MS/MS-Based Plasma Assay for Therapeutic Monitoring in Patients with APRT Deficiency**; Unnur A. Thorsteinsdottir[1]; Hrafnhildur L. Runolfsdottir[1]; Finnur F. Eiriksson[2]; Vidar O. Edvardsson[3]; Runolfur Palsson[1, 3]; Margret Thorsteinsdottir[1, 2]; *[1]University of Iceland, Reykjavik, Iceland; [2]ArcticMass, Reykjavik, Iceland; [3]Landspitali -The National University Hospital of Iceland, Reykjavik, Iceland*

WP 046 **A comprehensive LC-MSMS method to quantitate key retinoids of the visual cycle**; Mark Zambrowski[1]; Chung-Yeh Wu[1]; Siyuaun Shen[1]; Yubin Qiu[1]; Jennifer Campbell[1]; Christopher Adams[1]; Dennis Rice[1]; *[1]Novartis Institutes for BioMedical, Cambridge, MA*

WP 047 **Targeted Method Package for Amino acid, Vitamins and Nucleotide Cell Culture Components**; Xiaoxia Wang[1]; Yi Liu[1]; Zhengwei Jia[1]; *[1]Waters Technologies (Shanghai) Co, Ltd, Shanghai, China*

WP 048 **A Multiple Reaction Monitoring (MRM) Approach to Investigate Macrophage Proteome**; Katarzyna Macur[1, 2]; Andrew Schissel[1]; Sarah Zieschang[1]; Emma Harwood[1]; Brenda Morsey[1]; Howard Fox[1]; Pawel Ciborowski[1]; *[1]University of Nebraska Medical Center, Omaha, NE; [2]Intercollegiate Faculty of Biotechnology University of Gdansk and Medical University of Gdansk, Gdansk, Poland*

WP 049   **A Validated LC-MS/MS Assay for the Quantitation of 2-HG in Human Plasma Using A Surrogate Analyte Approach**; Feng Yin[1]; Yonghua Ling[2]; Rohini Narayanaswamy[1]; Heidi Mangus[1]; Fumin Li[2]; Hua Yang[1]; Guowen Liu[1]; [1]*Agios Pharmaceuticals, Inc., Cambridge, MA;* [2]*PPD, Middleton, WI*

WP 050   **High Throughput Quantitation of Human Milk Oligosaccharides in Breast Milk Samples Yields Variation from Geographically Diverse Sites**; Anita Vinjamuri[1]; Jasmine Davis[1]; Juan J. Castillo[1]; Carlito B Lebrilla[1]; [1]*UC Davis, Davis, CA*

WP 051   **Increasing the Ease of Use and Robustness of Nanoflow with Plug and Play Low Flow Source**; Arianna I Jones[1]; Christie Hunter[2]; Thomas Vander Schans[3]; Saghar Kaabinejadian[3]; Ken Jackson[3]; Curtis Mcmurtrey[3]; [1]*SCIEX, Framingham, MA;* [2]*SCIEX, Redwood Shores, California 1201;* [3]*Pure MHC, Oklahoma City, OK*

WP 052   **Global & targeted proteomic analysis reveals the presence of distinct proteomic signatures associated with Skull base vs Supratentorial meningiomas**; Shuvolina Mukherjee[1]; Deeptarup Biswas[2]; Aliasgar Moiyadi[3]; Sridhar Epari[3]; Sanjeeva Srivastava[1]; [1]*Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, India;* [2]*Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, Maharashtra, India, Mumbai, India;* [3]*Department of Pathology, Tata Memorial Centre, Mumbai, Dr. E Borges Road, Parel, Mumbai, India*

WP 053   **Rapid development and verification of pharmacodynamic proteomic-biomarkers of Achondroplasia in non-human primate cynomolgus macaques based on in-house human discovery-proteomics data**; Mahmud Hossain[1]; Wen Tang[1]; Yves Sabbagh[1]; Bailin Zhang[1]; [1]*Sanofi Genzyme, Framingham, MA*

WP 054   **Urinary Proteomics Reveals Putative Biomarkers Associated with Renal Function in Pediatric Patients with Ureteropelvic Junction Obstruction**; Dijana Vitko[1]; Shannon E. DiMartino[1]; Tanya Logvinenko[1]; Hsin-Hsiao Wang[1]; John W. Froehlich[1]; Richard S. Lee[1]; [1]*Boston Children's Hospital, Boston*

WP 055   **A mass spectrometry-based approach for quantifying low-level products of prohormone processing in human plasma**; Yinyin Ye[1]; Adam C. Swensen[1]; Yuqian Gao[1]; Thomas Fillmore[1]; Tujin Shi[1]; Wei-Jun Qian[1]; [1]*Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington*

WP 057   **Efficient Separation and Identification of 33-mer Gliadin Peptide and its Various Deamidated Forms Using Ultra-high-resolution LC/MS**; Jie Pu[1]; Chao Xue[1]; Matthew Szapacs[2]; Thomas Angel[2]; Jun Qu[1]; [1]*SUNY at Buffalo, Buffalo, NY;* [2]*GSK, Collegeville, PA*

WP 059   **Multi-Omic Biomarkers of Cellular Senescence**; Nathan Basisty[1]; Abhijit Kale[1]; Chisaka Kuehnemann[1]; Samah Shah[1]; Toshiko Tanaka[2]; Vagisha Sharma[3]; Luigi Ferrucci[2]; Judith Campisi[1, 4]; Birgit Schilling[1]; [1]*The Buck Institute for Research on Aging, Novato, CA;* [2]*Intramural Research Program of the National Institute on Aging, NIH, Baltimore, Maryland;* [3]*University of Washington, Seattle, WA;* [4]*Lawrence Berkeley Laboratory, University of California, Berkeley, California*

WP 060   **Deeper Kinome Coverage Using Multi-inhibitor Enrichment and Trapped Ion Mobility Mass Spectrometry**; Robert Sprung[1]; Petra Erdmann-Gilmore[1]; Michael East[2]; Gary L Johnson[2]; R Reid Townsend[1]; [1]*Washington University School of Medicine, St. Louis, MO;* [2]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 061   **Comparing whole blood lysates to Dried Blood Spots in targeted LC-MS/MS Proteomic Methods to detect markers of autologous blood transfusion**; Matt Kuruc[1]; Swapan Roy[1]; Johan Jakobsson[2]; Raik Wagner[2]; Christer Malm[2]; [1]*Biotech Support Group LLC, Monmouth Junction, NJ;* [2]*Pro Test Diagnostics AB, Umeå, Sweden*

**BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING II
WP 062-084**

WP 062   **In-gel cross-linking mass spectrometry (IGX-MS) benefits the analysis of distinctive protein complexes in selectivity and sensitivity**; Marie V. Lukassen[1]; Johannes F. Hevler[1]; Albert J.R. Heck[1]; [1]*Biomolecular Mass Spectrometry and Proteomics, Utrecht Institute for pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands*

WP 063   **Investigation of Noncovalent Interactions Between Peptides with Potential Intrinsic Sequence Patterns by Mass Spectrometry**; Chuan-Fan Ding[1]; Shutong Yang[2]; Qi Guo[2]; Fangling Wu[1]; Yuhong Wang[1]; [1]*Ningbo University, Ningbo, China;* [2]*Fudan University, Shanghai, China*

WP 065   **Systematic evaluation of amphiphilic structure environments on protein modification by fast photochemical oxidation of proteins**; Zhi Cheng[1]; Joshua Sharp[1]; [1]*University of Mississippi, Oxford, MS*

WP 066   **Fast and highly efficient affinity enrichment of Azide-A-DSBSO cross-linked peptides from a complex matrix**; Manuel Matzinger[1]; Wolfgang Kandioller[2]; Philipp Doppler[3]; Elke H Heiss[4]; Karl Mechtler[1, 5]; [1]*Institute of Molecular Pathology (IMP), Vienna BioCenter (VBC), Vienna, Austria;* [2]*Institute of Inorganic Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria;* [3]*Institute of Chemical, Environmental and Bioscience Engineering, Vienna University of Technology, Vienna, Austria;* [4]*Department of Pharmacognosy, Faculty of Life Sciences, University of Vienna, Vienna, Austria;* [5]*Institute of Molecular Biotechnology, Austrian Academy of Sciences (IMBA), Vienna BioCenter (VBC), Vienna, Austria*

WP 067   **Single nucleotide resolution Protein-RNA cross-linking/MS: Simple extension of the CLIR-MS workflow**; Michael Götze[1]; Chris P. Sarnowski[1]; Anna Knörlein[1]; Jonathan Hall[1]; Ruedi Aebersold[1]; Alexander Leitner[1]; [1]*ETH Zurich, Zurich, Switzerland*

WP 069   **Structural Study of Neural Cadherin Dimerization**; Anter A. Shami[1]; Addison E. Roush[1]; Samantha Davila[1]; Peilu Liu[2, 3]; Alan G. Marshall[2, 3]; Shana V. Stoddard[4]; Joshua S. Sharp[1]; Susan Pedigo[1]; [1]*University of Mississippi, University, MS;* [2]*Florida State University, Tallahassee, FL;* [3]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [4]*Rhodes College, Memphis, TN*

WP 070   **Characterizing calmodulin and small conductance calcium-activated potassium channel peptide interactions using chemical cross-linking coupled with UVPD and HCD**; Aarti Bashyal[1]; David Brent Halling[1]; Stephanie Liu[1]; Richard W Aldrich[1]; Carlos R Biaz[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 071   **A novel protocol for modeling protein structure using chemical cross-linking distance constraints**; Amanda M Cordibello[1]; Daniel P Farrell[2]; Leandro Martínez[1]; Frank Dimaio[2]; Fábio C Gozzo[1]; [1]*Universidade Estadual de Campinas, Campinas, Brazil;* [2]*University of Washington, Seattle, WA*

WP 072   **Novel Dual Cleavable Crosslinking Technology (DUCCT) with enrichment tags for confident identification of protein structures and protein interactions**; Akash Talukder[1]; Jayanta K. Chakrabarty[1, 2]; Saiful M. Chowdhury[1]; [1]*University of Texas at Arlington, Arlington, TX;* [2]*Columbia University, New York, NY*

WP 074   **Novel Methods for Chemical Crosslinking Based Protein Complex Analysis**; Qun Zhao[1, 2]; Yuxin An[2, 3, 4]; Lili Zhao[2, 3, 4]; Hang Gao[2, 3, 4]; Lihua Zhang[2, 3]; Yukui Zhang[2, 3]; [1]*Dalian Institute of Chemical Physics, ACS, Dalian, China;* [2]*CAS Key Laboratory of Separation Science for Analytical Chemistry, National Chromatographic R. & A. Center, Dalian, China;* [3]*Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China;* [4]*University of Chinese Academy of Sciences, Beijing,China, China*

WP 075   **Mapping interaction interfaces in S. erythraea DEBS1 complex**; Valeria Scorsato[1]; Bruno Cesar Amaral[1]; Juliana Helena Costa Smetana[2]; Fábio Cesar Gozzo[1]; [1]*University of Campinas, Campinas, Brazil;* [2]*Brazilian National Laboratory for Biosciences, Center for Research in Energy and Materials, Campinas, Brazil*

WP 076   **The Effect of Protein-Protein Interactions on the Pre-amyloid Structural Change of β-2-microglobulin as Measured by Covalent Labeling Mass Spectrometry**; Blaise Arden[1]; Richard W Vachet[1]; [1]*University of Massachusetts Amherst, Amherst, MA*

WP 077   **Protein-ligand interactions and restoration of age-related mitochondrial dysfunction**; James Bruce[1]; Juan D. Chavez[1]; Xiaoting Tang[1]; Matthew D. Campbell[1]; Gustavo Reyes[1]; Philip A. Kramer[1]; Rudy Stuppard[1]; Andrew Keller[1]; David J. Marcinek[1]; [1]*University of Washington, Seattle, WA*

WP 078   **Development of isobaric quantitative protein interaction reporter technology for comparative interactome studies**; Juan Chavez[1]; Andrew Keller[1]; Jared P. Mohr[1]; Jimmy K Eng[1]; James E Bruce[1]; [1]*University of Washington, Seattle, WA*

WP 079   **xiWORKFLOW: Taking Crosslinking Mass Spectrometry from Experiment to Insight**; Lutz Fischer[1]; Colin Combe[2]; Lars Kolbowski[1]; Martin Graham[2]; Juri Rappsilber[1, 2]; [1]*TU-Berlin, Berlin, Germany;* [2]*University of Edinburgh, Edinburgh, United Kingdom*

WP 080   **Improved FDR estimation of cross-linked peptides using PeptideProphet and Kojak**; Michael R. Hoopmann[1]; David D. Shteynberg[1]; Alex Zelter[2]; Trisha N. Davis[2]; Robert L. Moritz[1]; [1]*Institute for Systems Biology, Seattle, WA;* [2]*University of Washington, Seattle, WA*

WP 081   **Mass Spectrometry-Based Protein Footprinting Probes the Conformational Changes during Aβ42 Aggregation upon Binding to Novel Small Molecule Inhibitors**; Saketh Chemuru[1]; George Mathai[2]; Austin B. Moyle[1]; Don L. Rempel[1]; Liang Sun[3]; Liviu M Mirica[3]; Michael L. Gross[1]; [1]*Washington University, St Louis, MO;* [2]*Department of Chemistry, Sacred Heart College, Kochi, India;* [3]*Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL*

WP 083   **QUIN-XL: An approach for characterization of protein conformers by using cross-linking mass spectrometry and pattern recognition**; Louise Ulrich Kurt[1]; Milan Avila Clasen[2]; Marlon Dias Mariano Dos Santos[2]; Diogo Borges Lima[3]; Fabio Cesar Gozzo[4]; Paulo Costa Carvalho[2]; [1]*Carlos Chagas Institute, Fiocruz-PR, Curitiba, Brazil;* [2]*Fiocruz - PR, Carlos Chagas Institute, Curitiba, Brazil;* [3]*Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria;* [4]*University of Campinas, Campinas, Brazil*

WP 084   **X-ray Footprinting at Advanced Light Source (ALS)**; Sayan Gupta[1]; Matthew Rosi[2]; Brandon Russell[2]; Shawn Costello[3]; Line Kristensen[1]; Yan Chen[1]; Christopher J. Petzold[1]; Daniel P Deponte[4]; Corie Y Ralston[1]; [1]*Lawrence Berkeley National Laboratory, Berkeley;* [2]*Sonoma State University, Rohnert Park, California;* [3]*UC Berkeley, Berkeley, CA;* [4]*SLAC National Accelerator Laboratory, Melno Park, California*

CLINICAL ANALYSIS II
WP 085-109

WP 085 **Performance of serum apolipoprotein E measurement in EQA program with targets by isotope dilution LC-MS/MS**; Qing Li[1]; Yi Ju[1]; Zhonggan Jin[1]; Hewei Sun[1]; [1]*shanghai center for clinical laboratory, shanghai, China*

WP 086 **A High-Resolution Liquid Chromatography-Mass Spectrometry Method for Identification of Toxic Natural Products in Clinical Cases**; Y. Ruben Luo[1]; Robert Goodnough[2]; Kate Comstock[3]; Cassandra Yun[1]; Kara L Lynch[1]; [1]*University of California San Francisco, San Francisco, CA;* [2]*Baylor College of Medicine, Houston, TX;* [3]*Thermo Fisher Scientific, San Jose, CA*

WP 087 **Matrix effects-free determination of fentanyl in biological samples with Bio-SPME using a modified microfluidic open interface coupled to LEI-MSMS**; Priscilla Rocío Bautista[1]; Giorgio Famiglini[2]; Veronica Termopoli[2]; Pierangela Palma[2, 3]; Emir Nazdrajić[4]; Janusz Pawliszyn[4]; Achille Cappiello[2, 3]; [1]*University of Parma, Parma, Italy;* [2]*University of Urbino, Urbino, Italy;* [3]*Vancouver Island University, Nanaimo, BC;* [4]*University of Waterloo, Waterloo, ON*

WP 088 **HPLC-MS/MS determination of cyclosporine A concentrations in pediatric patientsundergoing HSCT and the relationship between cyclosporin**; Ziyi Yang[1]; Lei Wang[1]; Jianping Zhang[1]; Ying Zhao[2]; Hongxing Liu[1, 3, 4]; [1]*HebeiYanda Lu Daopei Hospital, Langfang, China, China;* [2]*Hebei Yanda Lu Daopei Hospital, Langfang, China, China;* [3]*Beijing Lu Daopei Institute of Hematology, Beijing, China;* [4]*Beijing Lu Daopei Hospital, Beijing, China*

WP 089 **Quantitative Urinalysis for Drugs of Abuse and their Metabolites using Paper Spray Mass Spectrometry (PS-MS) for Clinical and Forensic Toxicology**; Scott A. Borden[1, 2]; Armin Saatchi[1]; Jan Palaty[3]; Erik T. Krogh[1, 2]; Christopher G. Gill[1, 2, 4, 5]; [1]*Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC;* [2]*University of Victoria, Victoria, British Columbia;* [3]*Lifelabs Medical Laboratories, Burnaby, BC;* [4]*Simon Fraser University, Burnaby, BC;* [5]*University of Washington, Seattle, WA*

WP 090 **An Innovative Approach to Absolute Bioavailability Assessment with Strategic Isotopic labelling Optimization Using LC-MS/MS**; Hsinpin Ho[1]; David Marchisin[1]; Huidong Gu[1]; Todd Lusk[2]; Raj Mangaraj[2]; Wenying Li[1]; John Brailsford[1]; Anjaneya Chimalakonda[1]; Jim Shen[1]; [1]*Bristol-Myers Squibb, Princeton, NJ;* [2]*Q2 Solutions, Ithaca, NY*

WP 091 **Analysis of the Contrast Dye Iohexol in Human Serum using PaperSpray Technology**; Yu Zhu[1]; Katherine Walker[1]; Neloni Wijeratne[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

WP 092 **Selection of Peptide Targets for Clinical Measurements of Calprotectin and Lactoferrin in Stool**; Anthony Maus[1]; Kari Gurtner[1]; Jose Jara Aguirre[1]; Santosh Renuse[1]; Akhilesh Pandey[1]; Melissa Snyder[1]; [1]*Mayo Clinic, Rochester, MN*

WP 093 **Optimization and Quantitation of Antibiotics in Dried Plasma Spots Utilizing Paper Spray Mass Spectrometry**; Christine Skaggs[1]; Nicholas Manicke[1, 2]; Neloni Wijeratne[3]; Lindsey Kirkpatrick[4]; [1]*Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN;* [2]*Forensics and Investigative Sciences, Indiana University-Purdue University Indianapolis, Indianapolis, IN;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Department of Pediatrics, Division of Pediatric Infectious Diseases, Indiana University School of Medicine, Indianapolis, IN*

WP 094 **LC-MS/MS Analysis of Stratum Corneum on Skin Tape Strips – Current Development Towards Diagnostics of Endotypes of Atopic Diseases**; Evgeny Berdyshev[1]; Irina Bronova[1]; Elena Goleva[1]; Donald YM Leung[1]; [1]*National Jewish Health, Denver, CO*

WP 095 **Probe ElectroSpray Ionization for breast cancer rapid identification**; Enrico Davoli[1]; Silvia Giordano[2]; Hidekazu Saiki[3]; Takaaki Hiraoka[4]; Rita De Sanctis[5]; Rosalba Torrisi[5]; Daniela Pistillo[5]; [1]*Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy;* [2]*Shimadzu Italia SRL, Milano, Italy;* [3]*Shimadzu Corporation, Kyoto, Japan;* [4]*Shimadzu Europa GmbH, Duisburg, Germany;* [5]*Humanitas Clinical and Research Center – IRCCS, Milano, Italy*

WP 097 **Towards a point-of-care method to quantify tenofovir diphosphate in human whole blood for adherence monitoring**; Sangeeta Pandey[1]; Fan Pu[1]; Lane R. Bushman[2]; Peter L. Anderson[2]; Zheng Ouyang[1, 3]; R. Graham Cooks[1]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN;* [2]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado Denver, Aurora, CO 80045;* [3]*Department of Precision Instrument, Tsinghua University, Beijing, China*

WP 098 **Multiplex quantification of immunomodulatory proteins in tissue and plasma using targeted MRM mass spectrometry**; Jeff Whiteaker[1]; Lei Zhao[1]; Jacob Kennedy[1]; Regine Schoenherr[1]; Richard Ivey[1]; Julia Voytovich[1]; Amanda G Paulovich[1]; [1]*Fred Hutchinson Cancer Research Center, Seattle, WA*

WP 099 **Protective mechanism of dried blood spheroids**; Benji Frey[1]; Deidre E. Damon[1]; Danyelle M. Allen[1]; Jill Baker[1]; Sam Asamoah[1]; Abraham K. Badu-Tawiah[1]; [1]*The Ohio State University, Columbus, OH*

WP 100 **A comprehensive label-free proteomic profiling of medulloblastoma Group-3 tumors**; Manubhai Kp[1]; Anurag Kumar[1]; Deeptarup Biswas[1]; Epari Sridhar[2]; Aliasgar Moiyadi[2]; Neelam Shirsat[3]; Sanjeeva Srivastava[1]; [1]*IIT Bombay, Mumbai, India;* [2]*Tata Memorial Center (Hospital), Mumbai, India;* [3]*ACTREC, Mumbai, India*

WP 101   **An antibody-free LC-MS/MS method for the quantification of intact IGF-1 and IGF-2**; Mark S Pratt[1]; Martijn Van Faassen[1]; Noah Remmelts[1]; Rainer Bischoff[2]; Ido P Kema[1]; [1]*Department of Laboratory Medicine, University Medical Center Groningen, University of Groningen, Groningen, Netherlands;* [2]*Analytical Biochemistry, Department of Pharmacy, University of Groningen, Groningen, Netherlands*

WP 102   **Identification and Interlaboratory Validation of Endogenous Mouse Liver Peptides for Quality Control of Data Independent Acquisition MS-based Proteomics**; Huanhuan Gao[1]; Fangfei Zhang[1]; Shuang Liang[1]; Qiushi Zhang[1]; Yi Zhu[1]; Tianan Guo[1]; [1]*Westlake University, Hangzhou, China*

WP 103   **Human Histones Characterization using LC-TIMS-TOF MS**; Khoa Ngoc Pham[1]; Cesar E. Ramirez[1]; Yasir Mamun[1]; Francisco Alberto Fernandez-Lima[1]; [1]*Florida International University, Miami, FL*

WP 104   **Analysis of dexamethasone and 6-OH dexamethasone in rabbit plasma, aqueous and vitreous humors, and retinaby UHPLC-MS/MS**; Jianghong Gu[1]; Jiang Wang[1]; Ashok Chockalingam[1]; Lin Xu[1]; Sharron Stewart[1]; Yan Wang[1]; Patrick Faustino[1]; Diaa Shakleya[1]; [1]*FDA, Silver Spring, MD*

WP 105   **In vivo Proximity Labeling for Cell-type Specific Proteomics**; Sydney N Sunna[1]; Sruti Rayaprolu[1]; Ranjita Betarbet[1]; Hailian Xiao[1]; Lihong Cheng[1]; Allan Levey[1]; Nicholas T Seyfried[1]; Srikant Rangaraju[1]; [1]*Emory University, Atlanta, GA*

WP 106   **Identification of Metabolic Markers of Treatment Response and Adaptive Metabolic Changes in Ovarian Cancer Tissues using Mass Spectrometry Imaging**; Sunil P Badal[1]; Marta Sans[2]; Sanghoon Lee[3]; Sara Corvigno[3]; John Lin[4]; Michael Keating[4]; Jinsong Liu[3]; Anil Sood[3]; Livia Eberlin[4]; [1]*University of Texas at Austin, Austin, TX;* [2]*University of Texas at Austin, Austin, Texas;* [3]*The University of Texas MD Anderson Cancer Center, Houston, TX;* [4]*University of Texas Austin, Austin, TX*

WP 107   **Simultaneous determination of 24-hour urinary 5-hydroxyindoleacetic acid (5-HIAA), vanillylmandelic acid (VMA) and homovanillic acid (HVA) by LC-MS/MS for clinical testing**; Difei Sun[1]; Danijela Konforte[1]; Dawn-Marie Murphy Mclean[1]; Jan Palaty[2]; [1]*Lifelabs Medical Laboratories, Toronto, ON;* [2]*Lifelabs Medical Laboratories, Burnaby, BC*

WP 108   **Tumorous cell percentage determination by ambient molecular profiling of glial tumors**; Stanislav Pekov[1, 2]; Denis Bormotov[1, 2]; Pavel Nikitin[3]; Vasiliy Eliferov[1]; Vsevolod Shurkhay[1, 3]; Alexander Potapov[3]; Eugene Nikolaev[4]; Anatoly Sorokin[1]; Igor Popov[1, 3]; [1]*Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation;* [2]*V.L. Talrose Institute for Energy Problems of Chemical Physics, N.N. Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, Moscow, Russia;* [3]*N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia;* [4]*Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation*

WP 109   **A Rapid and Sensitive UPLC-MS/MS Assay for Simultaneous Quantitation of Vitamin A, B1, B6, and K in Human Blood/Plasma**; Gang Xu[1]; Brian Slay[1]; Nikolina Babic[1]; [1]*Department of Pathology and Laboratory Medicine, Medical University of South Carolina, Charleston, South Carolina*

CORPORATE POSTERS III
WP 110-112

WP 110   **Bruker at ASMS 2020: MALDI II for dramatic sensitivity improvements in SpatialOMx workflows, Bruker Daltonics**

WP 111   **Analytical Intelligence in the Digital Age of Mass Spectrometry, Shimadzu Scientific Instruments**

WP 112   **Orbitrap Exploris Mass Spectrometry, Thermo Fisher Scientific**

DRUG AND METABOLITE ANALYSIS
WP 113-136

WP 113   **A new method for improving LC-TOF/MS detection limits using simultaneous ion counting and waveform averaging**; Yousuke Kawai[1]; Yumi Miyake[2]; Toshinobu Hondo[2, 3]; Jean-Luc Lehmann[4]; Kentaro Terada[1, 2]; Michisato Toyoda[2]; [1]*Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Japan;* [2]*Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Toyonaka, Japan;* [3]*MS-Cheminformatics, Inabe-gun, Japan;* [4]*Acqiris SA, Geneva, Switzerland*

WP 115   **Applications of Til4 as a Diagnostic Reagent for the Detection of Sulfoxide-containing Metabolites or Impurities of Pharmaceuticals using UHPLC-HR/MS**; Li-Kang Zhang[1]; Ping Chen[1]; Hong Li[1]; Douglas Richardson[1]; [1]*Merck Research Laboratories, Kenilworth, NJ*

WP 116   **Determination of N-nitrosodimethylamine in metformin hydrochloride sustained-release tablets by LC-MS / MS**; Yong Wang; *shimadzu(china) C0.,LTD, Beijing, China*

WP 117   **Electrolytically regenerated suppressor introduced for addressing the non-MS compatible mobile phase challenges: GTP impurities identification as a case study**; Guoqiang Liu[1]; Da Chen[1]; Niusheng Xu[1]; [1]*Thermo Fisher Scientific, Shanghai, China*

WP 118 **Predicting the Future - Heading off Bioanalytical Issues with Two Solutions for Small Molecule In Vivo Quantitation**; Rachael K Bridgman; *AbbVie, North Chicago, IL*

WP 120 **High Resolution LC/MS Database Search Capability Across Multiple LC/MS Vendor Platforms Using a Custom Interface Program**; Michael P Mawn[1]; Jeff Gilbert[2]; Chris Brown[2]; Yelena Adelfinskaya[2]; Jeffrie Godbey[2]; Jesse Balcer[2]; *[1]Corteva Agriscience, Newark, DE; [2]Corteva Agriscience, Indianapolis, IN*

WP 121 **LC-APCI-dMRM Method for Quantitation of Eight Nitrosamine Impurities in ARB Drugs**; Raghavi Kakarla[1]; Tim Andres Marzan[1]; Jingyue Yang[1]; *[1]FDA, Saint Louis, MO*

WP 122 **Development of Rapid Analytical Screening Methods by Thermal Desorption-Electrospray Ionization/Mass Spectrometry (TD-ESI/MS) for Novel Oral Anticoagulants (NOACs)**; Yu-Ming Hsu[1]; Tzu-Yu Pan[1]; Chia-Fang Wu[1]; Ming-Tsang Wu[1, 2, 3, 4]; *[1]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [2]Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung, Taiwan; [3]Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan; [4]PhD Program of Environmental and Occupational Medicine and Graduate Institute of Clinical Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan*

WP 123 **Simultaneous analysis of novel oral anticoagulants in human urine by ultrasound-assisted salt-induced liquid-liquid microextraction coupled with liquid chromatography-tandem mass spectrometry**; Tzu-Yu Pan[1]; Sih-Syuan Li[1]; Yu-Ming Hsu[1]; Ming-Tsang Wu[1, 2, 3, 4]; Chia-Fang Wu[1]; *[1]Research Center for Environmental Medicine, Kaohsiung Medical University, Taiwan; [2]Ph.D. Program in Environmental and Occupational Medicine, Kaohsiung Medical University, Taiwan; [3]Graduate Institute of Clinical Medicine, Kaohsiung Medical University, Taiwan; [4]Department of Community Medicine,Kaohsiung Medical University Hospital, Kaohsiung Medical University, Taiwan*

WP 124 **Simultaneous quantitation of dexamethasone and dexamethasone phosphate in mice plasma and organ tissue by triple quadrupole LC-MS/MS with isotope dilution**; Michelle L Spruill[1]; Howard Martin[2]; Xinli Liu[1]; *[1]University of Houston College of Pharmacy, Houston, TX; [2]Sagis Diagnostics, Houston, TX*

WP 125 **Hydrogen/Deuterium and 16O/18O exchange mass spectrometry can boost the reliability of the compound identification**; Yury Kostyukevich[1]; Oxana Kovaleva[1]; Alexander Zherebker[1]; Eugene (evgeny) Nikolaev[2]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

WP 126 **Routine, ultra-trace analysis of nitrosamines in drugs using Gas Chromatography – Orbitrap Mass Spectrometry**; Dominic Roberts[1]; Giulia Riccardino[2]; Cristian Cojocariu[2]; Aaron Lamb[2]; Jason Cole[3]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Runcorn, United Kingdom; [3]Thermo Fisher Scientific, Austin, TX*

WP 127 **UV-Photodissociation on a hybrid QqLIT mass spectrometer to increase selectivity in LC Analysis**; Yves Le Blanc[1]; Mircea Guna[2]; Jeff Gilbert[3]; *[1]SCIEX, Concord, On, ON; [2]SCIEX, Concord, ontario; [3]Corteva Agriscience, Indianapolis, IN*

WP 128 **Unraveling the Gut Microbiome's Direct and Indirect Effects on Human Drug Metabolism**; Alan K. Jarmusch[1]; Alison Vrbanac[2]; Jeremiah D. Momper[3]; Joseph D. Ma[3]; Maher Alhaja[3]; Marlon Liyanage[3]; Rob Knight[2, 4, 5]; Shirley M. Tsunoda[3]; Pieter C. Dorrestein[1, 2, 4]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences and Collaborative Mass Spectrometry Innovation Center, University of California, San Diego, La Jolla, CA; [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]Center for Microbiome Innovation, University of California San Diego, La Jolla, California; [5]Department of Computer Science and Engineering, University of California, San Diego, La Jolla, CA*

WP 129 **Equine in vivo metabolites of the selective androgen receptor modulators (SARMs) LGD-3033 and ACP-105 determined using high-resolution mass spectrometry**; Malin Nilsson Broberg[1]; Heather Knych[2]; Ulf Bondesson[1]; Curt Pettersson[1]; Börje Tidstedt[3]; Scott Stanley[4]; Mario Thevis[5]; Mikael Hedeland[1, 3]; *[1]Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden; [2]Kenneth L. Maddy Equine Analytical Pharmacology Laboratory, School of Veterinary Medicine, University of California, Davis, CA; [3]National Veterinary Institute (SVA), Uppsala, Sweden; [4]University of Kentucky, Gluck Equine Research Center, Lexington, KY; [5]German Sport University, Centre for Preventive Doping Research, Cologne, Germany*

WP 130 **Structure identification of glyoxylate and cyanide reaction products by mass spectrometry**; Xu Shi; *Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA*

WP 131 **In vitro AmpC-mediated hydrolysis of β-lactams and the rapid detection of downstream metabolites by LC-MS/MS**; Anthony M. Haag[1, 2]; Thomas D. Horvath[1, 2]; Sigmund J. Haidacher[1, 2]; Kathleen M. Hoch[1, 2]; Jennifer K. Spinler[1, 2]; *[1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital - Microbiome Center, Houston, TX*

WP 132   **Pharmacokinetics of fluoxetine in horse**; Charles Veltri[1]; Laura Waitt-Wolker[2]; Krista Pearman[3]; Maria Lozoya[1]; Jeffrey W. Norris[3]; [1]*Midwestern University College of Pharmacy-Glendale, Glendale, AZ; [2]Midwestern University College of Veterinary Medicine, Glendale, AZ; [3]Midwestern University College of Graduate Studies, Glendale, AZ*

WP 133   **An Automated Approach to Urine Sample Preparation Employing Room Temperature Enzymatic Hydrolysis**; Jeremy Smith[1]; Jillian Neifeld[1]; Elena Gairloch[1]; [1]*Biotage, LLC, Charlotte, NC*

WP 134   **Measuring relevant markers in the place they matter: metabolomics of cerebrospinal fluid for better pediatric brain tumor therapy**; Boryana Petrova; *Boston Childrens Hospital, Boston, MA*

WP 135   **A Modified Quadrupole-Orbitrap Mass Spectrometer with Novel Data Acquisition Features Enhances Confident Metabolite Identification and Structure Elucidation**; Min Jiang[1]; Min Du[2]; Kate Comstock[2]; [1]*Amgen Inc., South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, California*

WP 136   **Mass spectrometric investigation and theoretical modeling of triazole complexes with amino acids**; Alisa Tokareva[1]; Vitaliy Chagovets[1]; Alexey Kononikhin; Natalia Starodubtseva[1]; Vladimir Frankevich[1]; [1]*FSBI «National Medical Research Center for Obstetrics, Gynecology and Perinatology Named After Academician V.I.Kulakov» Ministry Of Healthcare of the Russian Federation, Moscow, Russia*

EDUCATION: TEACHING MS AND TEACHING WITH MS
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WP 137   **A Course Undergraduate Research Experience (CURE) Featuring Peptide Mass Spectrometry**; Jay G Forsythe[1]; Michael W Giuliano[1]; [1]*College of Charleston, Charleston, SC*

WP 138   **Rapid Trypsin Digest for Peptide Analysis and Protein Identification in a Classroom Laboratory by MALDI-TOF**; Matthew A Portis[1]; Alexander D. Jacobs[1]; [1]*University of Florida, Gainesville, FL*

WP 139   **Build, Weigh, and Eat Molecules - Scalable Activities Coupled with Breath Analysis Using Direct Analysis in Real Time Mass Spectrometry**; Curtis Mowry; *Sandia National Laboratories, Albuquerque, NM*

ENERGY: BIOFUELS AND ALGAE
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WP 140   **Analytical tools for the speciation analysis in biocrudes**; Victor Garcia-Montoto[1, 2]; Sylvain Verdier[3]; Jan H Christensen[2]; Brice Bouyssiere[1]; [1]*University of Pau and Pays de l'Adour, CNRS, UMR5254, IPREM, Pau, France; [2]University of Copenhagen, Frederiksberg, Denmark; [3]Haldor Topsoe A/S, Lyngby, Denmark*

WP 141   **Inhibition of TOR in Chlamydomonas reinhardtii Leads to Rapid Cysteine Oxidation Reflecting Sustained Physiological Changes**; Amanda L. Smythers[1]; Megan M. Ford[1]; Evan W. Mcconnell[1]; Sarah C. Lowery[1]; Derrick R.J. Kolling[2]; Leslie M. Hicks[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Marshall University, Huntington, WV*

ENERGY: PETROLEUM AND BIOFUELS
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WP 142   **Distinguishing Routes of Gas-Phase Pyrolysis of Sulfonated Phenethyl Phenyl Ethers Using Collision-Induced Dissociation Mass Spectrometry**; Cory J Conder[1]; Sabyasachy Mistry[1]; Paul G Wenthold[1]; [1]*Purdue University, West Lafayette, IN*

WP 143   **KairosMS: A solution for complex mixture data analysis and visualisation**; Hugh E. Jones[1]; Remy Gavard[1]; Diana Catalina Palacio Lozano[1]; Mary J. Thomas[1]; Mark P. Barrow[1]; [1]*University of Warwick, Coventry, United Kingdom*

WP 144   **Energy-resolved MCAD of Seven Isomeric n-Pentylquinoline Radical Cations**; Yuyang Zhang[1]; Haoran Lei[1]; Hilkka I. Kenttämaa[1]; [1]*Purdue University, West Lafayette, IN*

WP 145   **Characterization of hydrodeoxygenated bio-oils by Fourier transform ion cyclotron mass spectrometry**; Timo Kekäläinen[1]; Idoia Hita Del Olmo[2]; Tómas Cordero Lanzac[3]; Gift Ogechukwu Okafor[1]; Pedro Castaño[2, 3]; Janne Jänis[1]; [1]*University of Eastern Finland, Joensuu, Finland; [2]Multiscale Reaction Engineering, KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia; [3]Department of Chemical Engineering, University of the Basque Country UPV/EHU, Bilbao, Spain*

WP 146   **Polymer modified bitumen investigated with direct insertion probe Fourier transform ion cyclotron resonance mass spectrometry**; Oscar Lacroix-Andrivet[1, 2]; Clément Castilla[1]; Christopher P. Rüger[1, 3]; Anna Luiza Mendes Siqueira[2]; Marie Hubert-Roux[1]; Carlos Afonso[1]; [1]*University of Rouen-Normandy, Mont-Saint-Aignan, France; [2]Total, Marketing Services, Research Center, Solaize, France; [3]University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany*

WP 147   **Effects of Oil and Gas Extraction on Drinking Water: Measuring Priority DBPs in Hydraulic Fracturing Impacted Waters**; Dallas G. Abraham[1]; Hannah K. Liberatore[2]; Michael J. Plewa[3]; Elizabeth D. Wagner[3]; Susan D. Richardson[1]; [1]*University of South Carolina, Columbia, SC; [2]US Environmental Protection Agency,, Raleigh, NC; [3]University of Illinois at Urbana-Champaign, Urbana, IL*

ENVIRONMENTAL: EXPOSOMICS
WP 148-153

WP 148	**Integration between chemical proteomics and lipidomics reveals a novel mechanism of MEHP in lipid accumulation via inhibiting fatty acid oxidation**; Mingliang Fang; *Nanyang Technological University, Singapore, Singapore*
WP 149	**Holistic approach for comprehensive xeno-metabolome coverage of Zebrafish embryos exposed to benzotriazoles, combining orthogonal chromatographic modes and Trapped-Ion-Mobility-QTOF**; Dimitrios E Damalas[1]; Elena I. Panagopoulou[1]; Adamantia Agalou[2]; Dimitris Beis[2]; Carsten Baessmann[3]; Artem Filipenko[4]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Athens, Greece; [2]Biomedical Research Foundation Academy of Athens, Athens, Greece; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Bruker Daltonics, Billerica, MA*
WP 150	**Detecting Novel Per- and Polyfluoroalkyl Substances in Water Supplies and Blood Using Non-targeted LC-IMS-MS Approaches**; Makayla R Foster[1]; James N. Dodds[1]; Molly T. Soper-Hopper[2]; Markace Rainey[3]; Facundo M. Fernandez[3]; Erin S. Baker[1]; *[1]Department of Chemistry, North Carolina State University, Raleigh, North Carolina; [2]Department of Chemistry, Northern Kentucky University, Highland Heights, Kentucky; [3]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia*
WP 151	**A rapid and efficient method for the extraction of per- and polyfluoroalkyl substances from plasma**; Bianca F. Silva[1]; Juan J. Aristizabal-Henao[1]; John A. Bowden[1]; *[1]University of Florida, Gainesville, FL*
WP 152	**Profiling Exposure-Dependent Protein Destabilization Through the Proxy of Hsp40 Affinity**; Joseph Genereux[1]; Guy Quanrud[2]; Maureen R Montoya[2]; *[1]University of California, Riverside, Riverside, CA; [2]University of California, Riverside, CA*
WP 153	**Development of analytical methods for exposomics research with deciduous teeth**; Sangwon Cha; *HUFS, Yongin, South Korea*

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WP 154	**Development of DNA Adductome Mass Spectral Database**; Jingshu Guo[1]; Robert J. Turesky[1]; Anamary Tarifa[2]; Anthony P. De Caprio[2]; Marcus S. Cooke[2]; Scott J. Walmsley[1]; Peter W. Villalta[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Florida International University, Miami, Florida*
WP 155	**Profiling serum metabolites, nutrients, and toxins in an exposomic investigation of the Isle of Wight multigenerational birth cohort**; Thilani M Anthony[1]; Wilfred J. J. Karmaus[2]; Su Chen[3]; Susan Ewart[4]; Syed Hasan Arshad[5, 6, 7]; John W. Holloway[8]; Hongmei Zhang[2]; A. Daniel Jones[9]; *[1]Michigan State University, East Lansing, MI; [2]Division of Epidemiology, Biostatistics, and Environmental Health, School of Public Health, University of Memphis, Memphis, Tennessee; [3]Department of Mathematical Sciences, University of Memphis, Memphis, Tennessee; [4]Department of Large Animal Clinical Sciences, College of Veterinary Medicine, Michigan State University, East Lansing, Michigan; [5]Clinical and Experimental Sciences, Faculty of Medicine, University of Southampton, Southampton, United Kingdom; [6]The David Hide Asthma and Allergy Research Centre, Isle of Wight, United Kingdom; [7]NIHR Respiratory Biomedical Research Unit, University Hospital Southampton, Southampton, United Kingdom; [8]Human Development and Health, University of Southampton, Southampton, United Kingdom; [9]Department of Biochemistry & Molecular Biology, Michigan State University, East Lansing, Michigan*
WP 156	**Top-down Proteomics Reveals Alterations in Liver Protein Profiles of C57Bl/6 Mice Exposed to Traffic-generated Emissions and a High Fat Diet**; Leah J Schneider[1]; Rachel Koerber[1]; Joann Lucero[1]; Jake Mcdonald[2]; Amie K. Lund[1]; *[1]University of North Texas, Denton, TX; [2]Lovelace Biomedical, Albuquerque, NM*
WP 157	**Monitoring of exogenous compound kinetics in exhaled breath**; Tanja Zivkovic Semren[1]; Csaba Laszlo[1]; Marta Gomez[2]; Guillermo Vidal-de-Miguel[2]; Julia Hoeng[1]; Manuel Peitsch[1]; Nikolai Ivanov[1]; Philippe A. Guy[1]; *[1]Philip Morris Products SA, Neuchatel, Switzerland; [2]Fossil Ion Technology, Madrid, Spain*
WP 158	**Repurposing Public Metabolomics Datasets for Construction of an Exposomics Spectral Library**; Biswapriya Biswavas Misra; *Independent Researcher, Namburu, India*

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WP 159	**Survey of Antibiotic Residues in Dried Distiller's Grains with Solubles from 14 Different States by LCMS**; Kevin R Tucker[1]; Samantha A Olendorff[1]; Karolina Chmielewska[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*
WP 160	**Determination of Coumarin in Smokeless Tobacco Products by UHPLC Coupled with Isotope Dilution Tandem Mass Spectrometry**; Jingcun Wu[1]; Erasmus Cudjoe[1]; Tyrally Ordinario[1]; SHENG-SUAN (victor) Cai[2]; Feng Qin[1]; *[1]PerkinElmer Inc., Woodbridge, ON; [2]Perkin Elmer, Waltham, MA*

WP 161   **Rapid Quantitation of Veterinary Dyes in Salmon Extracts Using PaperSpray Coupled with a TSQ Altis MS**; Neloni R Wijeratne[1]; Katherine Walker[1]; Ed George[1]; Laura E Burns[2]; Dwayne E Schrunk[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Iowa State University, Ames, IA*

WP 162   **Real-Time Chemical Puff Profiling of ENDS Aerosol with Chemical Ionization - Mass Spectrometry**; Alessandra Paul[1]; Devon O'regan[1]; Jeremy Nowak[1]; Luca Cappellin[2]; Nadja Heine[1]; *[1]JUUL Labs, San Francisco, CA; [2]Tofwerk, Thun, Switzerland*

WP 163   **Highly sensitive analysis of glyphosate, glufosinate and AMPA in the tap water and the beverages by LC-MS/MS without derivatization**; Kota Ishioka[1]; Miho Kawashima[2]; Manami Kobayashi[1]; Junichi Masuda[1]; Yoshihiro Hayakawa[2]; *[1]Shimadzu Corporation, Hadano, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

WP 164   **Quantitative measurement of pesticide residues in food by using high-throughput GC-MS/MS with a large volume inlet and fast GC condition**; Junkei Kou[1]; Kiotaka Konuma[1]; Kirk R. Jensen[2]; John Gonzales[2]; Kazuaki Murayama[1]; Yoshihisa Ueda[1]; *[1]JEOL Ltd, Akishima, Japan; [2]JEOL USA, Inc., Peabody, MA*

WP 165   **Classifying the pesticides in foods between GC-amenable and LC-amenable using the prediction model with molecular descriptors**; Takeshi Serino[1, 2]; Yoshizumi Takigawa[1]; Takeshi Otsuka[1]; Sadao Nakamura[1]; Tarun Anumol[3]; Shigehiko Kanaya[2]; *[1]Agilent Technologies, Hachioji, Japan; [2]Nara Institute of Science and Technology, Ikoma, Japan; [3]Agilent Technologies, Wilmington, DE19720*

WP 166   **An Alternate Workflow using Automated In-Line Pigment Removal for the Analysis of Multi-Residue Pesticides in Spinach by LC-MS/MS**; Sharon Lupo[1]; Randy Romesberg[1]; Xiaoning Lu[1]; *[1]Restek, Bellefonte, PA*

WP 167   **Determination of phthalate contamination onto plastic wrapped cucumbers using MALDI MS imaging**; Phoebe Bray[1]; Catherine Duckett[1]; Robert Bradshaw[1]; *[1]BMRC, Sheffield Hallam University, Sheffield, United Kingdom*

WP 168   **Rapid, High Sensitivity Analysis of Three Biotoxins Causing Diarrheic Shellfish Poisoning (Okadaic Acid, Dinophysistoxin-1 and Dinophysistoxin-2) in Mussel by UHPLC-MS/MS**; Sheng-Suan (victor) Cai; *PerkinElmer, Inc., San Jose, CA*

WP 169   **Fast Multiresidue Pesticide analysis using a modified quadrupole-Orbitrap mass spectrometer for quantitation and screening by FSddMS2 and DIA.**; Dipankar Ghosh[1]; Amadeo Fernández-Alba[2]; Łukasz Rajski[2]; Charles T. Yang[1]; Olaf Scheibner[3]; Christian Klaas[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]UNIVERSIDAD DE ALMERÍA, Almeria, Spain; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 170   **Evaluation of food processing methods in removing pesticide residues in celery – LC/Q-TOF MS analysis**; Yaoling Long[1]; Ebony Kia Thornton[1]; *[1]SCSU, Orangeburg, SC*

WP 171   **An end-to-end LC-MS/MS total workflow solution for quick and easy quantitative analysis of multiclass veterinary drug residues in meat**; Siji Joseph[1]; Aimei Zou[1]; Limian Zhao[2]; Ruben Garnica[2]; Dan-Hui-Dorothy Yang[3]; Patrick Batoon[3]; Chee-Sian Gan[1]; *[1]Agilent Technologies Singapore (Sales) Pte Ltd, Singapore, Singapore; [2]Agilent Technologies, Wilmington, DE19720; [3]Agilent Technologies, Santa Clara, CA*

WP 172   **USB Powered Coated Blade Spray Ion Source for future on-site food testing by portable Mass Spectrometry**; Marco Blokland[1]; Josha Jager[1]; Arjen Gerssen[1]; Janusz Pawliszyn[2]; Michel Nielen[1, 3]; *[1]Wageningen Food Safety research, Wageningen, Netherlands; [2]University of Waterloo, Waterloo, ON; [3]Wageningen University and Research, ORC, Wageningen, Netherlands*

WP 173   **Development of LC-MS/MS method for determination of microbial trans-glutaminase in food**; Irina Goncharova[1]; Zoya Nikiforova[1]; Elizaveta Goncharova[1]; Ilya Batov[1]; Denis Nekrasov[1]; Olga Ivanova[1]; Renat Selimov[1]; *[1]VGNKI, Moscow, Russia*

WP 174   **Characterization of Hemp-Based Consumer Products Using HS-GC/MS**; Jennifer Sanderson; *Agilent Technologies, Inc., Wilmington, DE*

WP 175   **Quantitative Analysis of Acrylamide in Peanut Butter using LC Triple Quadrupole Mass Spectrometry**; Yanan Yang[1]; Guannan Li[2]; Tina Chambers[2]; *[1]Agilent Technologies, Inc, Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA*

WP 176   **Determination of Phthalates in Food Reference Materials by Gas Chromatography-Tandem Mass Spectrometry (GC/MS/MS)**; Bruce A. Benner; *NIST, Gaithersburg, MD*

FORENSICS I
WP 177-192

WP 177   **Rapid detection of enhanced blood fingermarks recovered from various surfaces using MALDI MS and MSI**; Katie Kennedy[1]; Laura Cole[1]; Mark Sealey[2]; Simona Francese[1]; *[1]Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom; [2]Defence Science and Technology Laboratories (DSTL), Salisbury, United Kingdom*

WP 178 **Examining Transfer Efficiency of Paper Substrates Utilized as Physical Transfer Swabs**; Jessica M. Holtz[1]; Trevor J. McDaniel[1]; Alex Swiontek[1]; Christopher C. Mulligan[1]; [1]*Illinois State University, Normal, IL*

WP 179 **Development of an Updated Forensic DART-MS Mass Spectral Database**; Edward Sisco[1]; Arun Moorthy[2]; [1]*National Institute of Standards and Technology, Gaitherburg, MD;* [2]*National Institute of Standards and Technology, Gaithersburg, MD*

WP 180 **TIMS-qToF-MS for the investigation of electrochemically generated isomers of xenobiotics**; Oxana Korzhenko[1]; Uwe Karst[1]; [1]*University of Münster, Münster, Germany*

WP 181 **Identification of synthetic opioid analogs by high-resolution tandem mass spectrometry and machine learning**; Xinyi Sui[1]; Yufei Chen[1]; Nelson Vinueza[1]; [1]*North Carolina State University, Raleigh, NC*

WP 182 **Isobaric Drug Analyses Using Desorption Atmospheric Pressure Chemical Ionization and Online Derivatization**; Christopher M. Mcdonald[1]; Michael C Godwin[1]; Edgar Torres[1]; William Hoffmann[1]; [1]*Texas State University, San Marcos, TX*

WP 183 **Adhesive Tape Discrimination For Forensic Applications with Flowing Atmospheric Pressure Afterglow Ambient Mass Spectrometry**; Maureen E Oliva[1]; Dong Zhang[2]; Gerardo Gamez[2]; [1]*Texas Tech University, Lubbock, TX;* [2]*Texas Tech University, Lubbock, Texas*

WP 184 **Using DIA Analysis of Genetically Variant Peptides for Human Identification**; Paul A Rudnick[1]; Sanne Aalbers[2]; Daniel Chelsky[1]; Richard Johnson[2]; Brian Searle[3]; Bruce Weir[2]; Michael J MacCoss[2]; [1]*Spectragen Informatics, Bainbridge Island, WA;* [2]*University of Washington, Seattle, WA;* [3]*Institute for Systems Biology, Seattle, WA*

WP 185 **Protein-Based Body Fluid Identification: Specificity and Sensitivity**; B. Mckay Allred[1]; Glenn Kresge[1]; Henry Zheng[1]; [1]*Defense Forensic Science Center, Forest Park, GA*

WP 186 **Comparison of Sample Preparation Approaches for the Extraction of 11-nor-9-carboxy-Δ9-THC from Urine prior to GC/MS Analysis**; Rhys Jones[1]; Katie-Jo Teehan[1]; Lee Williams[1]; Geoff Davies[1]; Adam Senior[1]; Alan Edgington[1]; Helen Lodder[1]; Jillian Neifeld[2]; [1]*Biotage GB Limited, Cardiff, United Kingdom;* [2]*Biotage, Charlotte, North Carolina*

WP 187 **Matching Forensic Proteomic Profiles to Genetic Sequences through the Detection of Genetically Variable Peptides from Fingerprint Touch Samples**; Myles W Gardner[1]; F. Curtis Hewitt[1]; Michael A. Freitas[2]; August E. Woerner[3]; Alan R. Smith[1]; Andrew J. Reed[2]; Danielle S. LeSassier[1]; Liwen Zhang[2]; Kathleen Q. Schulte[1]; Maryam Baniasad[2]; Katharina Weber[1]; Leah W. Allen[1]; Megan E. Powals[1]; Benjamin C. Ludolph[1]; Benjamin Crysup[3]; Anthony D. Kappell[1]; [1]*Signature Science, LLC, Austin, TX;* [2]*The Ohio State University, Columbus, OH;* [3]*University of North Texas Health Science Center, Fort Worth, TX*

WP 188 **Spectral Library Search Based Method for the Confident Identification of Genetically Variant Peptides in Human Hair**; Zheng Zhang[1]; Meghan C. Burke[1]; William E. Wallace[1]; Yuxue Liang[1]; Sergey Sheetlin[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

WP 189 **Differentiation of Morphologically Similar Human Head Hairs from Two Demographically Similar Individuals Using Amino Acid Ratios and GC/MS**; Allison M Macri[1]; Robert H Powers[1]; Alyssa L M Marsico[1]; [1]*University of New Haven, West Haven, CT*

WP 190 **Analysis of Synthetic Cannabinoids in Plant Materials Using a LDTD-MS/MS System**; Sandra Imrazene[1]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; [1]*Phytronix Technologies, Quebec, QC*

WP 191 **Identification and Quantification of Metoprolol in Equine Plasma by LC-MS/MS**; Jaclyn R. Missanelli[1, 2]; Youwen You[1, 2]; Rachel M. Proctor[1, 2]; Mary A. Robinson[1, 2]; [1]*University of Pennsylvania, Kennett Square, PA;* [2]*PA Equine Toxicology and Research Laboratory, West Chester, PA*

WP 192 **Fingermark Sampling Using Particle Capture Mass Analysis with Nanoparticles**; Jamira Stephenson[1]; Kermit K Murray[1]; [1]*Louisiana State University, Baton Rouge, LA*

FUNDAMENTALS: ION SPECTROSCOPY
WP 193-200

WP 193 **UV-Vis Action Spectroscopy and Energetics of Charge-Tagged Adenosine Radicals**; Yue Liu[1]; Andy Dang[1]; František Tureček[1]; [1]*University of Washington, Seattle, WA*

WP 194 **REMPI and MATI spectroscopy of non-deuterated and deuterated m-chloro- and m-fluoropyridine**; Niklas Helle[1]; Jurgen Grotemeyer[1]; [1]*Christian-Albrechts-Univ, Kiel, Germany*

WP 195 **Differentiation of Hydroxyproline Isomers by Gas-Phase Infrared Ion Spectroscopy of Alkali Metal-Ion Complexes**; Baku Acharya[1]; Widana K D N Kaushalya[1]; Amanda Patrick[1]; [1]*Mississippi State University, Starkville, MS*

WP 196   **Infrared ion spectroscopy: an alternative for structure identification by NMR?**; Rianne Van Outersterp[1]; Jonathan Martens[1]; Giel Berden[1]; Valerie Koppen[2]; Jos Oomens[1]; Filip Cuyckens[2]; [1]*FELIX Laboratory, Radboud University, Nijmegen, Netherlands; [2]Janssen R&D, Beerse, Belgium*

WP 197   **Understanding the Wavelength Dependence for Photodissociation of Protonated Methylpyridines Within the UV Region**; Benjamin I. Mckinnon[1]; Samuel J.P. Marlton[1]; James P. Bezzina[1]; Stephen J. Blanksby[2]; Adam J. Trevitt[1]; [1]*University of Wollongong, Wollongong, Australia; [2]Queensland University of Technology, Brisbane, Australia*

WP 198   **Spectroscopic Identification of Gas-Phased Synthesized Nitrogen-Containing Polycyclic Aromatic Ions**; Oisin J. Shiels[1]; Samuel J.P. Marlton[1]; Patrick D. Kelly[1]; Jack Turner[1]; Stephen J. Blanksby[2]; Gabriel Da Silva[3]; Adam J. Trevitt[1]; [1]*School of Chemistry and Molecular, University of Wollongong, Wollongong, Australia; [2]Queensland University of Technology, Brisbane, Australia; [3]University of Melbourne, Parkville, Australia*

WP 199   **From isolated self-assembled peptides towards nanostructures: a mass-selective IR action spectroscopy study**; Iuliia Stroganova[1]; Sjors Bakels[1]; Anouk M. Rijs[1]; [1]*FELIX Laboratory, Radboud University, Nijmegen, Netherlands*

WP 200   **Rapid IR Spectroscopy and Ion-Packet Enrichment for glycan identification (9/20)**; Ali H Abikhodr[1]; Vasyl Yatsyna[1, 2]; Thomas R. Rizzo[1]; [1]*EPFL/LCPM, Lausanne, Switzerland; [2]University of Gothenburg, Gothenburg, Sweden*

FUNDAMENTALS: ION STRUCTURE/ENERGETICS
WP 201-212

WP 201   **Alkali Cation Size-Specific Guest Trapping in Supramolecular Complexes Characterized Using CRAFTI Collision Cross Sections**; Tina H. M. Farzan[1]; Mariah Pay[1]; Brigham Pope[1]; David V. Dearden[1]; [1]*Brigham Young University, Provo, UT*

WP 202   **Deprotonated Glycan Dissociation Chemistry**; Jordan M Rabus[1]; Benjamin J Bythell[1]; [1]*Ohio University, Athens, OH*

WP 203   **On the Observation of Isomers of Enterobactin and their Fate upon Binding FeIII: an Empirical and Theoretical Study**; Daryl Giblin[1]; Lindsey K. Steinberg[2]; Jan M. Crowley[2]; Michael L. Gross[1]; Jeffrey P. Henderson[2]; [1]*Washington University, St Louis, MO; [2]Washington University in St.Louis, St.Louis, MO*

WP 204   **Collision Cross-section Measurements of Precursor and Selected Fragmentation Products in Single Experiments by SORI – CRAFTI**; Andrew J. Arslanian[1]; Caleb Tinsley[1]; Noah Mismash[1]; David V. Dearden[1]; [1]*Brigham Young University, Provo, UT*

WP 205   **Investigating structural properties of single atom doped cobalt sulfide clusters through mass spectrometry**; Habib Gholipour-Ranjbar; *560 Oval Drive West Lafayette, Indiana 47907-2084, West Lafayette, IN*

WP 206   **Characterization of Potential Thioredoxin-Mimetic Peptides**; Michael D. Browne[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

WP 207   **Fragmentation pathways of transition metal substituted polyoxovanadates**; Solita Marie Wilson[1]; Ellen M. Matson[2]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN; [2]University of Rochester, Rochester, NY*

WP 208   **Rapid, quantitative investigation of gas-phase unfolding/dissociation activation enthalpies and entropies for native protein ions**; Micah T Donor[1]; Samantha O. Shepherd[1]; James S Prell[1]; [1]*University of Oregon, Eugene, OR*

WP 209   **Determining Topologies of Alkylammonium Complexes of Cucurbit[6]uril Using MultiCRAFTI and SORI-CID Techniques in an FTICR Mass Spectrometer**; Jamir Shrestha[1]; Caleb Tinsley[1]; Andrew J. Arslanian[1]; Zixuan Feng[2]; Tina H. M. Farzan[1]; Mariah Pay[1]; David V. Dearden[1]; [1]*Brigham Young University, Provo, UT; [2]Colorado State University, Fort Collins, CO*

WP 210   **Conformational and Thermochemical Changes of Cysteine Containing Peptides upon Chiral Inversion of Cysteine**; Yuntao Zhang[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

WP 211   **N-Acetyl Glycan Structure and Dissociation Chemistry**; Benjamin Bythell[1]; Shanshan Guan[1]; Jordan M Rabus[1]; Matthew Murphy[2]; John Tschampel[2]; [1]*Ohio University, Athens, OH; [2]University of Missouri, St. Louis, St. Louis, MO*

WP 212   **An Experimental and Computational Study of the Decompositon of [UO2(O2C-C≡C-CH3)(NO3)2]-** ; Luke Metzler[1]; Michael Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA*

FUNDAMENTALS: IONIZATION MECHANISMS
WP 213-220

WP 213   **Probing the Electrospray Source Conditions on the Protonation Isomer Distributions of Ciprofloxacin**; Boris Ucur[1]; Adam J. Trevitt[1]; Stephen J. Blanksby[2]; Ben I. Mckinnon[1]; Samuel J.P. Marlton[1]; [1]*School of Chemistry and Molecular Bioscience, Wollongong, Australia; [2]Queensland University of Technology, Brisbane, Australia*

WP 214   **Chemical modification of the matrix gas: Comparison experiments with ESI-MS and ESI-IMS-MS**; Christine Polaczek[1]; Christian Thoben[2]; Maria Allers[2]; Stefan Zimmermann[2]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany;* [2]*Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany*

WP 215   **Factors that affect the formation of multiply charged protein ions in a MALDI process**; Avinash Adhikrao Patil[1]; Thi Khanh Ly Lai[1]; Cheng-Kang Chiang[1]; Wen-Ping Peng[1]; [1]*National Dong Hwa University, Shoufeng, Taiwan*

WP 216   **Discrimination of position isomers of benzene derivatives based on TOF mass spectra derived using femtosecond laser ionization**; Kennosuke Hoshina[1]; Tatsuro Shirota[1]; [1]*Niigata University of Pharmacy and Applied Life Sciences, Niigata, Japan*

WP 217   **Towards Higher Throughput in LC-MS - DB-nESI Overcomes the Ion Flux Problem of Modern Instruments**; Sebastian Brandt[1]; Michael Schilling[1]; Albert Sickmann[1, 2, 3]; Joachim Franzke[1]; Stefan Loroch[4]; [1]*Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany;* [2]*Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany;* [3]*University of Aberdeen, Department of Chemistry, Aberdeen, United Kingdom;* [4]*Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany*

WP 218   **Microwave-Assisted Electrospray Ionization**; Steven Ray[1]; Maria Rivera[1]; [1]*University at Buffalo, SUNY, Buffalo, NY*

WP 219   **Influence of Matrix Crystal Size on the Plume Effective Temperature in MALDI**; Lee Elliott[1]; Gary R. Kinsel[2]; Mary E. Kinsel[2]; [1]*Southern Illinois University Carbondale, Carbondale;* [2]*Southern Illinois University Carbondale, Carbondale, IL*

WP 220   **New Insights Relative to Matrices in Mass Spectrometry**; Milan Pophristic[1]; Khoa Hoang[1]; Charles N Mcewen[1]; [1]*MSTM LLC, Newark, DE*

GC/MS: GENERAL
WP 221-229

WP 221   **Unexpected EI fragmentations: Loss of tetramethylsilane in vicinal TMS diols; Transfer of an acetyl group across an aromatic amino alcohol**; N. Rabe Andriamaharavo[1]; H. Martin Garraffo[1]; Stephen E. Stein[1]; [1]*National Institute of Standards and Technology, Gaithersburg, MD*

WP 222   **Rearrangement of TMS of halogenated 1-phenylethanone and related compounds in EI Mass Spectra**; Yufang Zheng[1]; H. Martin Garraffo[1]; Quan-Long Pu[1]; Weihua Ji[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

WP 223   **Rearrangement of the TMS ester of 4-Oxo-4H-chromene-2-carboxylic acid and analogs in EI mass spectra**; Quan-Long Pu[1]; H. Martin Garraffo[1]; Yufang Zheng[1]; N. Rabe Andriamaharavo[1]; Stephen E. Stein[1]; [1]*National Institute of Standards and Technology, Gaithersburg, Maryland*

WP 224   **Characterization of glycerides and other impurities in biodiesel by high temperature gas chromatography combined with isobutane chemical ionization mass spectrometry**; Roza Wojcik[1]; Tessa L Oxford[1]; Cherylyn W Wright[1]; Angela M Melville[1]; Bob W Wright[1]; [1]*PNNL, Richland, WA*

WP 225   **Thermal Desorption Coupled Gas Chromatography-Mass Spectrometry Analysis of Low Emission Polyurethane Foam for Automobile Applications**; Yujing Tan[1]; Adam Grzesiak[1]; Eric Pearce[1]; Gavin Marr[1]; Michael Donate[1]; Kelly Kiszka[1]; [1]*The Dow Chemical Company, Midland, MI*

WP 226   **Comparison of extracted and non-extracted calibration curves in the GC-MS determination of method detection limits for haloacetonitriles**; George William Kajjumba[1, 2]; Tammy Jones-Lepp[1, 2]; Meena Ejjada[1, 2]; Erica J Marti[1, 2]; [1]*University of Nevada, Las Vegas, Las Vegas, NV;* [2]*Department of Civil and Environmental Engineering and Construction, Las Vegas, NV*

WP 227   **Development and validation of an improved, TF-SPME based, standard gas generating vial for the repeatable generation of headspace standards**; Jonathan J Grandy[1]; Khaled Murtada[1]; João R Belinato[1, 2, 3]; Janusz Pawliszyn[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*Institute of Chemistry, University of Campinas, Campinas, Brazil;* [3]*National Institute of Science and Technology in Bioanalysis (INCTBio), Campinas, Brazil*

WP 228   **Inferring the molecular mass of an analyte from its electron ionization mass spectrum**; Arun S Moorthy[1]; Anthony J Kearsley[1]; W Gary Mallard[1]; William E Wallace[1]; Stephen E Stein[1]; [1]*NIST, Gaithersburg, MD*

WP 229   **Identification and quantification of the phytosterols in Korean maize (Zea mays L.) F1 hybrids using Gas Chromatography-mass spectrometry**; Dong Yeol Lee[1]; Won Min Jeong[1]; Hyeong Hwan Lee[1]; Jong Soo Ryu[2]; Tae Wook Jung[2]; Sang Gon Kim[1]; [1]*Gyeongnam Oriental Anti-Aging Institute, Sancheong-gun, South Korea;* [2]*National Institute of Crop Science, Miryang, South Korea*

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY
WP 230-246

WP 230 **Dual capillary-based vibrating sharp-edge spray ionization (cVSSI) with online solution-phase hydrogen deuterium exchange for distinguishing disaccharides and glycan isomers**; Sandra N Majuta[1]; Anthony Debastiani[1]; Sara Macios[1]; Kushani Attanayake[1]; Stephen J Valentine[1]; [1]*West Virginia University, Morgantown, WV*

WP 231 **Characterization of Reversible Protein-Protein Interactions (PPI) in High Concentration mAbs Using Hydrogen/Deuterium Exchange Mass Spectrometry (HDX-MS)**; Rajashekar Kammari[1]; Jainik P. Panchal[2]; Brent Kochert[3]; Smeet Deshmukh[2]; Elizabeth M. Topp[1]; [1]*Department of Industrial and Physical Pharmacy, College of Pharmacy, Purdue University, West Lafayette, IN;* [2]*Sterile Formulation Sciences, Merck & Co, Inc., Kenilworth, NJ;* [3]*AR&D Mass Spectrometry, Merck & Co. Inc., Kenilworth, NJ*

WP 232 **Organic Solvents on the HDX Platform for Efficient Denaturation**; Chunyang Guo[1]; Ming Cheng[2]; Lindsey K. Steinberg[3]; Jeffrey P. Henderson[4]; Michael L. Gross[4]; [1]*WUSTL, St. Louis, MO;* [2]*The Scripps Research Institute, La Jolla, CA;* [3]*Washington University in St.Louis, St.Louis, MO;* [4]*Washington University, St Louis, MO*

WP 233 **The Deuterium Calculator: An open-source software for hydrogen-deuterium exchange mass spectrometry analysis**; Thomas Welborn[1]; Kellye Cupp-Sutton[1]; Zhe Wang[1]; Si Wu[1]; Kenneth Smith[2]; [1]*University of Oklahoma, Norman, OK;* [2]*Oklahoma Medical Research Foundation, Oklahoma City, OK*

WP 234 **Preparation of a stably labeled mimic of a deuterated protein to evaluate mass measurement error in HX-MS experiments**; Ashley E. Grande[1]; David D. Weis[1]; [1]*University of Kansas, Lawrence, KS*

WP 235 **Hydrogen/deuterium exchange mass spectrometry (HDX-MS) for complex sample analysis**; Mulin Fang[1]; Zhe Wang[1]; Thomas Welborn[1]; Kellye A. Cupp-Sutton[1]; Kenneth Smith[2]; Si Wu[1]; [1]*University of Oklahoma, Norman, OK;* [2]*Oklahoma Medical Research Foundation, Oklahoma City, OK*

WP 236 **Supercharging for Improved ECD/ETD-Based Hydrogen/Deuterium Exchange Mass Spectrometry of Biotherapeutics**; Leeanne Wang[1]; Qingyi Wang[1]; Kristina Håkansson[1]; [1]*Department of Chemistry University of Michigan, Ann Arbor, MI*

WP 237 **Extracting all Protein Dynamics Information in Hydrogen/Deuterium Exchange Mass Spectrometry Data**; Zhongqi Zhang; *Amgen Inc., Thousand Oaks, CA*

WP 238 **Hydrogen/Deuterium Exchange-MS/MS of Carbohydrate-Metal Adducts to Track Structural Changes Based on Metal-Adduction**; H. Jamie Kim[1]; Darren T. Gass[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

WP 239 **OligoR: An online software suite for oligonucleotide HDX/MS and quantitative native MS data treatment and visualization**; Eric Largy[1]; Valérie Gabelica[1]; [1]*Université de Bordeaux, Pessac, France*

WP 240 **Interpretation of the Hydrogen-Deuterium Exchange Mass Spectrometry Structural Proteomics Data using Molecular Dynamics Simulations**; Evgeniy V. Petrotchenko[1]; Konstantin I. Popov[2]; Christoph H. Borchers[1, 3, 4]; [1]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [2]*Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC;* [3]*Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC;* [4]*Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

WP 241 **Imidazolium Compounds as Internal Exchange Reporters for Hydrogen/Deuterium Exchange by Mass Spectrometry**; Taylor A Murprhee[1]; Clint Vorauer[1]; Marie Brzoska[1]; Miklos Guttman[1]; [1]*University of Washington, Seattle, WA*

WP 242 **Fundamentals of Gas-Phase Hydrogen Deuterium Exchange (gHDX) and Implications for Structural Elucidation of Small Molecules**; Sanjit S. Uppal (Sunny)[1, 2]; Abhigya Mookherjee[1, 2]; Rick Harkewicz[1, 2]; Sarah E. Beasley[1, 2]; Matthew F. Bush[1, 3]; Miklos Guttman[1, 2]; [1]*University of Washington, Seattle, WA;* [2]*Department of Medicinal Chemistry, University of Washington, Seattle, WA;* [3]*Department of Chemistry, University of Washington, Seattle, WA*

WP 243 **Performance Evaluation of Hydrogen Deuterium Exchange on a Waters Synapt XS**; Lindsay Morrison[1]; Barbara J Sullivan[1]; [1]*Waters Corporation, Beverly, MA*

WP 244 **Avoiding hydrogen scrambling with minimal ion transmission loss for HDX-MS/MS-ETD analysis on a high-resolution Q-TOF mass spectrometer**; Daniel T. W. Wollenberg[1, 2]; Stuart Pengelley[3]; Jeppe C. Mouritsen[1]; Detlev Suckau[3]; Christian I. Jorgensen[1]; Thomas J. D. Jorgensen[2]; [1]*Novozymes A/S, Kgs. Lyngby, Denmark;* [2]*University of Southern Denmark, Odense M, Denmark;* [3]*Bruker Daltonic GmbH, Bremen, Germany*

WP 245 **In-electrospray H/D Exchange of Carbohydrates Using a D2O/N2Gas Infusion System**; Ana V. Quintero[1]; O. Tara Liyanage[1]; Chinthaka A. Seneviratne[2]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX;* [2]*Mass Spectrometry Center, Baylor University, Waco, TX*

WP 246 **HDXmodeller: an online webserver for high-resolution HDX-MS with auto-validation**; Antoni James Borysik[1]; Ramin Ekhteiari Salmas[1]; [1]*King's College London, London, United Kingdom*

IMAGING MS: INSTRUMENTATION
WP 247-258

WP 247   **Development of a Novel Ion Imaging Unit toward Microscope Mode Mass Spectrometry Imaging**; Tsuyoshi Hirao[1, 2]; Hajime Nishimura[2]; Yasuhide Naito[1]; [1]*The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan;* [2]*Hamamatsu Photonics K.K., Iwata, Japan*

WP 248   **Comparative N-glycome analysis of prostate cancer tissues using MALDI Q-TOF versus MALDI-FTICR imaging mass spectrometry workflows**; Grace Grimsley[1]; Connor A West[1]; Xiaowei Lu[1]; Anand S Mehta[1]; Peggi M Angel[1]; Richard R Drake[1]; [1]*Medical University of South Carolina, Charleston, SC*

WP 249   **Sub-micron 3D SIMS imaging combined with automated, high mass resolution MS/MS**; Alexander Pirkl[1]; Henrik Arlinghaus[2]; Daniel Breitenstein[3]; Karsten Lamann[4]; Elke Tallarek[3]; Birgit Hagenhoff[3]; Ewald Niehuis[1]; [1]*IONTOF Technologies GmbH, Muenster, Germany;* [2]*IONTOF Technologies GmbH, Muenster, Germany;* [3]*TASCON GmbH, Muenster, Germany;* [4]*TASCON GmbH, Muenster, Germany*

WP 250   **New insights into vitamin D metabolism and androgen intracrinology by on-tissue derivatization and novel MALDI-2-MS ion Mobility (timsTOF-fleX) mass spectrometry**; Diego F Cobice[1]; Jens Soltwisch[2, 3]; Bram Heijs[2, 4]; Annika Koch[5]; Karl Smith[6]; Klaus Dreisewerd[2, 3]; C. Logan Mackay[7]; [1]*Mass Spectrometry Centre, Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University,, Coleraine,, United Kingdom;* [2]*Institute of Hygiene, University of Muenster, Muenster, Germany;* [3]*Interdisciplinary Center for Clinical Research (IZKF), Muenster, Germany;* [4]*Center for Proteomics & Metabolomics, Leiden University Medical Center,, Leiden, Netherlands;* [5]*Bruker Daltonics, Bremen, Germany;* [6]*Mass Spectrometry Centre, Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University, Coleraine, United Kingdom;* [7]*SIRCAMS, Edinburgh, United Kingdom*

WP 251   **From Tissue Imaging to Cancer Surgery – Utilisation of Laser Desorption – Rapid Evaporative Ionisation Mass Spectrometry**; Daniel Simon[1]; Julia Abda[1]; Hanifa J.A. Koguna[1, 2]; Stefania M. Stavrakaki[1]; Olof Isberg[1]; Julia Balog[3]; Tamas Karancsi[3]; Josephine Bunch[1, 2]; Zoltan Takats[1]; [1]*Imperial College London, London, United Kingdom;* [2]*National Physical Laboratory, Teddington, United Kingdom;* [3]*Waters Research Center, Budapest, Hungary*

WP 252   **A Dual SIMS / MALDI Source for an Orthogonal TOF Imaging Mass Spectrometer**; Ian G. M. Anthony[1]; Joel D. Keelor[2]; Sebastian Böhm[3]; Shane R. Ellis[4]; Claus Köster[3]; Jens Hoehndorf[5]; Ron M.A Heeren[1]; [1]*Maastricht MultiModal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Limburg, Netherlands, Maastricht, Netherlands;* [2]*Amsterdam Scientific Instruments, Amsterdam, Netherlands;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*University of Wollongong, Wollongong, Australia;* [5]*Bruker Daltonik GmbH, Bremen, Germany*

WP 253   **Using Ozone-Induced dissociation to demonstrate varying distribution patterns of unsaturated Isobaric lipids by DESI imaging Mass Spectrometry**; Mark Towers[1]; Lisa Reid[1]; Berwyck Poad[2]; Martin Green[1]; Emmanuelle Claude[1]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Queensland University of Technology, Brisbane, Australia*

WP 255   **High-throughput ion microscope imaging using the time-stamping Timepix3 sensor**; Natasha M Smith[1]; Robert Burleigh[1]; Daniel Wood[1]; Ang Guo[1]; Michael Burt[1]; Ian Shipsey[1]; Daniela Bortoletto[1]; Richard Plackett[1]; Mark Brouard[1]; [1]*University of Oxford, Oxford, United Kingdom*

WP 256   **Design and characterization of novel sprayer for high resolution tissue imaging by desorption electrospray ionization (DESI)**; Stephen J Hattan[1]; Presha Rajbhandari[2]; Brandon Fowler[2]; Fereshteh Zandkarimi[2]; Brent R. Stockwell[2]; Gregory Roman[1]; Wade Leveille[1]; Jeffrey Musacchio[1]; Ashwin Meyyappan[1]; Jim Murphy[1]; Joseph Michienzi[1]; Emrys Jones[3]; Steven Pringle[3]; [1]*Waters Corporation, Milford, Massachusetts;* [2]*Columbia University, New York, NY;* [3]*Waters Corporation, Wilmslow, United Kingdom*

WP 257   **Development of a Multimodal Fully Integrated Imaging Platform using Infrared Laser-Assisted REIMS and DESI for High Throughput Slide analysis**; Istvan Pap[1]; Richard Schaffer[1]; Csaba Hajdu[1]; Daniel Simon[2]; Tamas Karancsi[1]; Julia Balog[1]; [1]*Waters Research Center, Budapest, Hungary;* [2]*Imperial College London, London, United Kingdom*

WP 258   **Desorption Electrospray Ionisation Imaging on the Cyclic Ion Mobility-Mass Spectrometry System**; Emrys A Jones[1, 2]; Matthew Gentry[2]; Jakub Ujma[1]; Robert Tonge[1]; Danielle Mcdougall[2]; James I Langridge[1]; Adam Mcmahon[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*University of Manchester, Manchester, United Kingdom*

IMAGING MS: PHARMACEUTICALS, METABOLITES, AND LIPIDS I
WP 259-277

WP 259   **MALD-MSI Evaluation of Penetration of Different Pyrazole-based Compounds into Multicellular Tumor Spheroids**; Yijia Wang[1]; Yong Ai[2]; Fengtian Xue[2]; Amanda B. Hummon[1]; [1]*The Ohio State University, Columbus, OH;* [2]*University of Maryland School of Pharmacy, Baltimore, MD*

WP 260   **Non-targeted exploration of metabolic processes and xenobiotic metabolism in plants exposed to micropollutants using mass spectrometry imaging**; Claire Villette[1]; Alexandre Verdue[2]; Aiko Barsch[2]; Nikolas

Kessler[2]; <u>Shannon Cornett</u>[3]; Loïc Maurer[1, 4]; Dimitri Heintz[1]; *[1]Plant Imaging and Mass Spectrometry (PIMS), Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, Strasbourg, France; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA; [4]Département Mécanique, ICube Laboratoire des sciences de l'ingénieur, de l'informatique et de l'imagerie, Strasbourg, France*

WP 261   **The absorption of drugs through porcine gastrointestinal tissue analysed by mass spectrometry imaging**; <u>Chloe E Spencer</u>[1]; Stephen Rumbelow[2]; Steven Mellor[3]; Catherine Duckett[1]; Malcolm R Clench[1]; *[1]BMRC, Sheffield Hallam University, Sheffield, United Kingdom; [2]CRODA Inc (B88), New Castle, DE19720; [3]CRODA Europe Ltd, Leek, United Kingdom*

WP 262   **4D-Lipidomics based automated annotation of MALDI Imaging data using a dedicated bioinformatics pipeline**; <u>Janina Oetjen</u>[1]; Christian Marsching[2]; Sven W. Meyer[1]; Corinna Henkel[1]; Annika Koch[1]; Nikolas Kessler[1]; Wiebke Timm[1]; Aiko Barsch[1]; Jan H. Kobarg[1]; Dennis Trede[1]; Heiko Neuweger[1]; Carsten Hopf[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim Technical University, Mannheim, Germany*

WP 263   **Effect of COX-inhibition on the lipid change in early pregnancy in mice**; <u>Éva Szabó</u>[1]; Stefania Gitta[1]; Janos Schmidt[1]; Laszlo Mark[1]; *[1]Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary*

WP 264   **MALDI Mass Spectrometry Imaging of Gemcitabine Treatment in Pancreatic Cancer: Exploring Multiple Matrices to See the Whole Picture**; <u>Caitlin Tressler</u>[1]; Hong Liang[1]; Katherine Stumpo[2]; James R. Eshleman[1]; Kristine Glunde[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, Maryland; [2]University of Scranton, Scranton, PA*

WP 265   **Mass Spectrometry Imaging to Evaluate the Role of Sulfatide in NeuroHIV**; <u>Daniela D'amico</u>[1]; Eliseo Eugenin[1]; Brendan Prideaux[1]; *[1]UTMB, Galveston, TX*

WP 266   **Understanding Mitragyna speciosa alkaloid metabolism and pharmacology in rat brain using imaging mass spectrometry**; <u>Zhongling Liang</u>[1]; Orélia Cerlati[1]; Tamara I. King[2]; Abhisheak Sharma[2]; Christopher R. Mccurdy[2]; Boone M. Prentice[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of Florida, Gainesville, FL*

WP 267   **Lipid Distribution in Liver Is Disrupted in the Translocator Protein (TSPO, 18-KDa) Knockout Mouse Model**; <u>Cristina I Silvescu</u>[1]; Li Yuchang[2]; Chantal Sottas[2]; Junji Watanabe[2]; Jeremy Wolff[1]; Shannon Cornett[1]; Vassilios Papadopoulos[2]; *[1]Bruker Scientific LLC, Billerica, MA; [2]School of Pharmacy, University of Southern California, Los Angeles, CA*

WP 268   **Metabolite Explorer: a software tool for targeted analysis of mass spectrometry imaging data**; Thomas Moerman[1]; Michael Becker[2]; <u>Nico Verbeeck</u>[1, 3]; Marc Claesen[1, 3]; *[1]Aspect Analytics NV, Genk, Belgium; [2]Boehringer Ingelheim Pharma GmbH, Biberach a.d. Riss, Germany; [3]KU Leuven, ESAT-STADIUS, Leuven, Belgium*

WP 269   **Analysis of Novel Bioproduct Pathways in Populations of Arthrospira Platensis at Microorganism Resolution**; <u>Peter V Shanta</u>[1]; Steven M Rowland[1]; Lieve M.L. Laurens[1]; *[1]National Renewable Energy Laboratory, Golden, Colorado*

WP 271   **A study of drug metabolism using a zebrafish larvae model and MALDI-MS Imaging**; Yu Mi Park[1, 2]; Jennifer Herrmann[3, 4]; Daniel Krug[1, 4]; Aiko Barsch[5]; <u>Nikolas Kessler</u>[5]; Alice Ly[6]; Jan H. Kobarg[6]; Rolf Müller[3, 4]; *[1]Department of Microbial Natural Products, Helmholtz-Institute for Pharmaceutical Research Saarland (HIPS), Helmholtz Centre for Infection Research (HZI) and Department of Pharmacy, Saarland University, Saarbrücken, Germany; [2]Environmental Safety Group, Korea Institute of Science and Technology (KIST) Europe, Saarbrücken, Germany; [3]Department of Microbial Natural Products, Helmholtz-Institute for Pharmaceutical Research Saarland (HIPS), Helmholtz Centre for Infection Research (HZI) and Department of Pharmacy, Saarland University,, Saarbrücken, Germany; [4]German Center for Infection Research (DZIF), Partner Site Hannover-Braunschweig, Braunschweig, Germany; [5]Bruker Daltonics, Bremen, Germany; [6]Bruker Daltonics, Bremen, Germany*

WP 272   **Laser post ionization (MALDI-2) coupled to a timsTOF fleX improves limits of detection for statin drug compounds in MALDI-MS imaging**; <u>Jan Schwenzfeier</u>[1]; Bram Heijs[2, 3]; Klaus Dreisewerd[2, 4]; Nana-Maria Wagner[5]; Jens Soltwisch[2, 4]; *[1]Institute for Hygiene, University of Muenster, Muenster, Germany; [2]Institute of Hygiene, University of Muenster, Muenster, Germany; [3]Center for Proteomics and Metabolomics, Leiden, Netherlands; [4]Interdisciplinary Center for Clinical Research (IZKF), Muenster, Germany; [5]Departments of*

WP 273   ***In situ* isobaric and isomeric lipid mapping and identification by MALDI-Ion Mobility Separation-Mass Spectrometry Imaging**; <u>Tingting Fu</u>[1]; Janina Oetjen[2]; Manuel Chapelle[2]; Alexandre Verdue[2]; Matthias Szesny[2]; Arnaud Chaumot[3]; Davide Degli-Esposti[3]; Olivier Geffard[3]; Yohann Clément[1]; Arnaud Salvador[1]; Nannan Tao[4]; Sophie Ayciriex[1]; *[1]Institut des Sciences Analytiques, Universite Claude Bernard, Villeurbanne, France; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Irstea, UR RiverLy, Laboratoire d'écotoxicologie, Villeurbanne, France; [4]Bruker Daltonics, San Jose, CA, United States*

WP 274   **High Throughput and High Sensitivity Isomer-resolved Imaging of Lipids by Integration of Ozone-induced dissociation with a MALDI-QTOF Mass Spectrometer**; <u>Andrew Bowman</u>[1]; Britt S. R. Claes[1]; Berwyck Poad[2];

Ron M.A Heeren[1]; Stephen J. Blanksby[2]; Shane R. Ellis[1, 3]; [1]*Maastricht MultiModal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Limburg, Netherlands, Maastricht, Netherlands;* [2]*Queensland University of Technology, Brisbane, Australia;* [3]*University of Wollongong, School of Chemistry and Molecular Bioscience, Wollongong, Australia*

WP 275   **Comprehensive analysis of metabolites and biomarkers in lung using MALDI-MSI and DESI-MSI**; William Temple Andrews[1]; Amanda Oglesby-Sherrouse[1]; Angela Wilks[1]; Ann M Farese[2]; Thomas J MacVittie[2]; Maureen A Kane[1]; [1]*University of Maryland School of Pharmacy, Baltimore, MD;* [2]*University of Maryland School of Medicine, Baltimore, Maryland*

WP 276   **Integrating high resolution MALDI imaging into the development pipeline of anti-Tuberculosis drugs**; Axel Treu[1]; Julia Kokesch-Himmelreich[1]; Alan Race[1]; Kerstin Walter[2]; Christoph Hölscher[2]; Andreas Römpp[1]; [1]*Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany;* [2]*Infection Immunology, Research Center Borstel, Borstel, Germany*

WP 277   **Visualization of Intact protein for the study of lithium neuropharmacology in mouse brain with MALDI - Imaging Mass Spectroscopy**; Yuki Yasui[1]; Kohta Yamamoto[2]; Daiki Kameyama[3]; Takashi Nirasawa[4]; Ryo Kajita[4]; Nobuto Kakuda[3]; Takafumi Hirata[2]; Masaya Ikegawa[3]; [1]*Doshisha University, Kyotanabe, Japan;* [2]*Geochemical Research Center, The University of Tokyo, Japan;* [3]*Doshisha University, Kyotanabe, Japan;* [4]*Bruker Japan K.K., Yokohama, Japan*

INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES
WP 278-303

WP 278   **Improvements to compareMS2 and new compareMS2GUI for measuring distances between LC-MS/MS datasets with applications from molecular phylogenetics to quality control**; Nino Vrolijk[1, 2]; Madhushri Shrikant Varunjikar[3]; Josef Daniel Rasinger[3]; Benjamin Neely[4, 5]; Magnus Palmblad[6]; [1]*Leiden University Medical Center, Leiden, Netherlands;* [2]*University of Applied Sciences, Leiden, Netherlands;* [3]*Institute of Marine Research, Bergen, Norway;* [4]*National Institute of Standards and Technology, Charleston, SC;* [5]*Hollings Marine Laboratory, Charleston, SC;* [6]*Leiden University Medical Center, Leiden, Netherlands*

WP 279   **LC-MS ESI Parameter Optimization with Bayesian Optimization for High Sensitivity Measurement**; Yusuke Tagawa[1]; Yuki Ishikawa[1]; Mikael Levi[1]; Wataru Fukui[1]; Jun Watanabe[1]; Hisanori Morita[1]; [1]*Shimadzu corporation, Kyoto, Japan*

WP 281   **A Novel Approach to Estimate Protein-Protein Interactions using Proteomics Data**; Ahmad Borzou[1]; Rovshan G. Sadygov[1]; [1]*UTMB, Galveston, TX*

WP 282   **EnvCNN: A Convolutional Neural Network Model for Evaluating Isotopomer Envelopes in Top-Down Mass-spectral Deconvolution**; Abdul Rehman Basharat[1]; Zhe Wang[2]; Rachele Lubeckyj[3]; Si Wu[2]; Liangliang Sun[3]; Xiaowen Liu[1]; [1]*Indiana University - Purdue University Indianapolis, Indianapolis, IN;* [2]*University of Oklahoma, Norman, OK;* [3]*Michigan State University, East Lansing, MI*

WP 283   **A new algorithm for fast, parameter-free extraction of ion chromatograms**; Rob Smith[1, 2]; Mathew Guiterrez[1, 2]; [1]*University of Montana, Missoula, MT;* [2]*Prime Labs, Inc., Missoula, MT*

WP 284   **LC-MS correspondence using a feature-aware, direct match approach without retention time alignment**; Michael Callahan[1, 2]; Rob Smith[1, 2]; [1]*Prime Labs, Inc., Missoula, MT;* [2]*University of Montana, Missoula, MT*

WP 285   **Identification of Cutibacterium acnesby machine learning using amino acid sequence information**; Tatsuki Okubo[1]; Kanae Teramoto[1]; Yoshihiro Yamada[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; [1]*Shimadzu corporation, Kyoto, Japan*

WP 286   **Fast deisotoping algorithm and its implementation in MSFragger search engine**; Guo Ci Teo[1]; Daniel Polasky[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

WP 287   **JUMPt: ordinarydifferential equation-based protein turnover modeling of mass spectrometric data from metabolically labeled animals**; Surendhar Reddy Chepyala[1]; Xueyan Liu[2]; Alex M. Breuer[1]; Zhiping Wu[1]; Ji-Hoon Cho[1]; Ariana Mancieri[1]; Yun Jiao[1]; Hui Zhang[3]; Junmin Peng[1]; [1]*St.Jude Children's Research Hospital, Memphis, TN;* [2]*University of New Orleans, New Orleans, LA;* [3]*Northwestern University, Chicago, IL*

WP 288   **PRiSM: exhaustive and agnostic database searching**; Joris Van Houtven[1]; Kurt Boonen[2]; Geert Baggerman[2]; Kris Laukens[3]; Jef Hooyberghs[4]; Dirk Valkenborg[1]; [1]*Hasselt University, Hasselt, Belgium;* [2]*Centre for Proteomics, Antwerpen, Belgium;* [3]*Biomina, Antwerpen, Belgium;* [4]*VITO, Mol, Belgium*

WP 289   **Peptide profiling and predictive modelling of dairy products throughout fermentation**; Fionnuala Murphy[1, 2, 3]; Stefan Clerens[1, 3, 4]; Esther Meenken[1]; Julie Dalziel[1, 3]; Joanne Hort[2, 3]; Julia Low[2, 3]; [1]*AgResearch, Christchurch, New Zealand;* [2]*Massey University, Palmerston North, New Zealand;* [3]*Riddet Institute (Massey University), Palmerston North, New Zealand;* [4]*Biomolecular Interaction Centre (Canterbury University), Christchurch, New Zealand*

WP 290   **Clustering of spectra renders improved, automated identification and quantification of glycan structures**; Christopher Ashwood[1]; Matthew The[2]; Rebekah L Gundry[1]; Lukas Kall[3]; [1]*CardiOmics Program, Center for Heart and Vascular Research; Division of Cardiovascular Medicine; and Department of Cellular and Integrative Physiology, University of Nebraska Medical Center, Omaha, NE, 68198;* [2]*Technical University of Munich (TUM), Freising, Germany;* [3]*Royal Institute of Technology, Stockholm, Sweden*

WP 291   **Floodlight and Searchlight: Innovative Software for Machine Learning Assisted Data Reduction and Pattern Analysis**; Kristin A Favela[1]; Michael J Hartnett[1]; Andrew J Schaub[1]; Jake A. Janssen[1]; Adam K Van Horn[1]; David W Vickers[1]; Keith S Pickens[1]; [1]*Southwest Research Institute, San Antonio, TX*

WP 292   **Mobilatron: software framework for signal extraction from ion mobility enabled mass spectrometry data**; Dmitry Avtonomov[1]; Sarah E. Haynes[1]; Daniel A. Polasky[1]; Carolina Rojas Ramirez[1]; Brandon T. Ruotolo[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

WP 293   **CoreMS: Open Source Mass Spectrometry Software Framework for Small Molecules Analysis**; Yuri E. Corilo[1]; Allison M. Thompson[1]; William Kew[1]; Lisa M Bramer[1]; Lee Ann McCue[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

WP 294   **Correctly controlling false discovery rates in targeted database searches**; Andy Lin[1]; Uri Keich[2]; William Stafford Noble[1]; [1]*University of Washington, Seattle, WA;* [2]*University of Sydney, Camperdown, Australia*

WP 295   **Improvements in Two-Dimensional GCxGC Data Alignment by a Supervised Learning Guided Approach for Automated Peak Comparisons**; <u>Andrew J Schaub</u>[1]; Jake A. Janssen[1]; Michael J Hartnett[1]; Kristin A Favela[1]; Adam K Van Horn[1]; David W Vickers[1]; Keith S Pickens[1]; [1]*Southwest Research Institute (SwRI), San Antonio, TX*

WP 296   **Accelerated Isotopic Envelope Calculations using IsoSpec**; <u>Michal P. Startek</u>[1]; Dirk Valkenborg[2]; Mateusz Krzysztof Lacki[3]; [1]*University of Warsaw, Warsaw, Poland; [2]Hasselt University, Hasselt, Belgium; [3]University Medical Center, Johannes Gutenberg University, Mainz, Germany*

WP 297   **MSstatsSampleSize: Simulation tool for optimal design of high-dimensional MS-based proteomics experiments**; <u>Ting Huang</u>[1]; Meena Choi[1]; Tiannan Guo[2]; Sumedh Ravikant Sankhe[1]; Yansheng Liu[3]; Matthew Tham[1]; Ruedi Aebersold[4, 5]; Olga Vitek[1]; [1]*Northeastern University, Boston, MA; [2]Westlake University, Hangzhou, China; [3]Yale University School of Medicine, West Haven, CT; [4]ETH Zurich, Zurich, Switzerland; [5]University of Zurich, Zurich, Switzerland*

WP 298   **Repository-scale queries of MS/MS spectra**; <u>Benjamin Pullman</u>[1]; Nuno Bandeira[1, 2]; [1]*UC San Diego, Ja Jolla, CA; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

WP 299   **A real-time dynamic data correction method for enhancing resolving power and spectral quality in mass spectrometry**; Chih-Hao Hsiao[1]; Yu-Meng Ou[1]; Shu-Yun Kuo[1]; <u>Yi-Sheng Wang</u>[1]; [1]*Genomics Research Center, Academia Sinica, Taipei, Taiwan*

WP 300   **Science Autonomy and the ExoMars Mission: Machine Learning to Help Find Life on Mars**; <u>Victoria Da Poian</u>[1]; Eric Lyness[1]; William B Brinckerhoff[1]; Ryan M. Danell[2]; Desmond Kaplan[3]; Xiang Li[4]; Melissa G. Trainer[1]; [1]*NASA Goddard Space Flight Center, Greenbelt, MD; [2]Danell Consulting, Inc., Winterville, NC; [3]KapScience LLC, TEWKSBURY, MA; [4]University of Maryland Baltimore County, Baltimore, Maryland*

WP 301   **Masserstein: A Python package for a robust linear deconvolution using optimal transport**; <u>Michal Ciach</u>[1]; Grzegorz Skoraczynski[1]; Szymon Majewski[2]; Michal P. Startek[1]; Blazej Miasojedow[1]; Dirk Valkenborg[3]; Anna Gambin[1]; [1]*University of Warsaw, Warsaw, Poland; [2]Institute of Mathematics, Polish Academy of Sciences, Warsaw, Poland; [3]Hasselt University, Hasselt, Belgium*

WP 302   **The MasSpOT - Optimal Transport for Mass Spectrometry**; <u>Grzegorz Skoraczynski</u>[1]; Blazej Miasojedow[1]; Szymon Majewski[2]; Anna Gambin[1]; [1]*Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; [2]Institute of Mathematics, Polish Academy of Sciences, Warsaw, Poland*

WP 303   **Utilizing conditional probability distributions to identify peptides that contain heavy isotopes**; <u>Jonathon O'brien</u>[1]; Phillip Seitzer[1]; Nicole Haste[1]; Celeste M. Sandoval[1]; Yao Wong[1]; Ramin Rad[1]; Aleksandr Gaun[1]; Carmela Sidrauski[1]; Vladimir Jojic[1]; Fiona E. Mcallister[1]; Bryson D. Bennett[1]; [1]*Calico Life Sciences LLC, South San Francisco, California*

INFORMATICS: MULTIOMICS INTEGRATION
WP 304-321

WP 304   **ProteomicsDB: Integrating drug targets, phenotypes and expression data**; <u>Patroklos Samaras</u>[1]; Tobias Schmidt[1]; Marwin Shraideh[2]; Ludwig Lautenbacher[1]; Martin Frejno[1]; Siegfried Gessulat[1]; Jana Zecha[1]; Anna Jarzab[1]; Maria Reinecke[1]; Stephanie Heinzlmeir[1]; Johannes Rank[2]; Helmut Krcmar[2]; Bernhard Kuster[1]; Mathias Wilhelm[1]; [1]*Technical University of Munich (TUM), Freising, Germany; [2]Technical University of Munich (TUM), Garching, Germany*

WP 305   **Comprehensive Proteogenomic Analysis of Peptides and Proteoforms with MetaMorpheus**; <u>Rachel M Miller</u>[1]; Anthony J. Cesnik[2, 3]; Robert J Millikin[1]; Michael R. Shortreed[1]; Lloyd M Smith[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin; [2]Stanford University, Stanford, CA; [3]Chan Zuckerber Biohub, San Francisco, CA*

WP 306   **Proteogenomics-driven synthetic lethality discovery to predict targetable protein dependencies induced by somatic deletions in breast cancer**; <u>Jonathan T Lei</u>[1]; Eric J Jaehnig[1]; Bing Zhang[1]; [1]*Baylor College of Medicine, Houston, TX*

WP 307   **Proteomic data commons: a resource for proteogenomic analysis**; <u>Ratna Rajesh Thangudu</u>[1]; Michael Holck[1]; Deepak Singhal[1]; Paul A Rudnick[2]; Michael J MacCoss[3]; Nathan J Edwards[4]; Karen A Ketchum[1]; Christopher R Kinsinger[5]; Erika Kim[5]; Anand Basu[1]; [1]*ESAC, Inc., Rockville, MD; [2]Spectragen Informatics, Bainbridge Island, WA; [3]University of Washington, Seattle, WA; [4]Georgetown Univ., Washington, DC; [5]National Cancer Institute, Bethesda, MD*

WP 308   **Integrative transcriptome, proteome, and phosphoproteome reveal new aspects of high productivity in CHO cells**; <u>Prashant Kaushik</u>[1]; Vijay Tejwani[2]; Shangzhong Li[3, 4]; Michael Henry[1]; Nathan E. Lewis[3, 4, 5]; Paula Meleady[1]; Susan T. Sharfstein[2]; [1]*National Institute for Cellular Biotechnology, Dublin City University, Dublin, Ireland; [2]Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, NY; [3]Department of Bioengineering, University of California, San Diego, La Jolla, CA; [4]Novo Nordisk Foundation Center for Biosustainability, University of California, San Diego, La Jolla, CA; [5]Department of Pediatrics, University of California, San Diego, San Diego, La Jolla, CA*

WP 309 **Multi-omics analysis for cancer stem cell-like acquisition properties derived by spheroid in polymer thin film induced-human ovarian cancer cells**; Hee-Sung Ahn[1]; Junhyuk Song[2]; Sunyoung Seo[3]; Jiyoung Yu[1]; Jeonghun Yeom[1]; Hyunggee Kim[4]; Sangyong Jon[5]; Kyunggon Kim[1, 6]; [1]*Asan Medical Center, Seoul, South Korea;* [2]*Korea Advanced Institute of Science and Technology, Deajeon, South Korea;* [3]*Korea University, Seoul, South Korea;* [4]*Korea University, Seoul, South Korea;* [5]*Korea Advanced Institute of Science and Technology, Daejeon, South Korea;* [6]*University of Ulsan, Seoul, South Korea*

WP 310 **Alomic : An Artificial Intelligence (AI) enabled integrative Omics pipeline**; Raghav Sehgal[1]; Qiushi Sun[1]; Rebecca Cardone[1]; Richard Martyn Williams[1]; Xiaojian Zhao[1]; Surbhi Poddar[2]; Richa Mudgal[2]; Richard Schneider[3]; Richard G. Kibbey[1]; [1]*Yale University, New Haven, CT;* [2]*Elucidata, Delhi, India;* [3]*NCATS/NIH, Rockville, MD*

WP 311 **Robust In Silico Fractionation of Diverse Molecular Ion Adduct Forms in Positive- and Negative-Ion Mode ESI**; Luke T. Richardson[1]; Shubhneet Warar[1]; Touradj Solouki[1]; [1]*Baylor University, Waco, TX*

WP 312 **Evaluating customized database generation methods for metaproteomics analysis**; Subina Mehta[1]; Thomas Mcgowan[1]; James E Johnson[1]; Praveen Kumar[1]; Magnus O Arntzen[2]; Francesco Delogu[2]; Marie A Crane[3]; Peter S Thuy-Boun[4]; Dennis W Wolan[4]; Timothy J Griffin[1]; Pratik Dilip Jagtap[1]; [1]*University of Minnesota, Minneapolis, MN/55455;* [2]*Norwegian University of Environmental and Life Sciences, Ås, Norway;* [3]*Macalester College: Private Liberal Arts College, St. Paul, Minnesota;* [4]*The Scripps Research Institute, La Jolla, CA*

WP 313 **ImmuNOVO: An integrated platform for neoantigen discovery based on immunopeptideomics and genomic data**; Sujun Li[1]; Yue Qi[2]; Udayan Guha[2]; Haixu Tang[1]; [1]*Indiana University, Bloomington, IN;* [2]*Thoracic & Gastrointestinal Oncology Branch, Center for Cancer Research, NCI, Bethesda, MD*

WP 314 **Integrated genome and metabolome analysis highlights the role of Glucagon-like Peptide 1 signaling and other pathways in increasingly severe asthma**; Jalal Siddiqui[1]; Tara Eicher[1]; Rachel Kelly[2]; Raghu Machiraju[1]; Juan Celedón[3]; Scott Weiss[2]; Jessica Lasky-Su[2]; Ewy Mathé[1]; [1]*The Ohio State University, Columbus, OH;* [2]*Brigham and Women's Hospital, Harvard Medical School, Boston, MA;* [3]*University of Pittsburgh, Pittsburgh, PA*

WP 315 **SysMet: A Suite of Tools for Integrative Systems Metabolomics**; Mohammad R Nezami-Ranjbar[1]; Linge Yan[1]; Habtom W Ressom[1]; [1]*OmicsCraft, Washington, District of Columbia*

WP 316 **Numerical and a priori knowledge-driven methods for integrating metabolomics data with other omics data**; Andrew Patt[1]; Tara Eicher[2]; Elizabeth Baskin[1]; Bofei Zhang[3]; Joseph Mcelroy[1]; Kevin Coombes[1]; Ewy Mathe[1]; [1]*Ohio State University Medical Center, Columbus, OH;* [2]*Ohio State University, Columbus, Ohio;* [3]*New York University School of Medicine, New York, New York*

WP 318 **Multi-omics investigation of synergistic effects of Traditional Chinese Medicine herbal decoction on cultured osteoblasts**; Kenneth Kin-Leung Kwan[1]; Ben Tin-Yan Wong[2]; Anna Xiao-Dan Yu[1]; Tina Ting-Xia Dong[1]; Henry Hei-Ning Lam[2]; Karl Wah-Keung Tsim[1]; [1]*Division of Life Science and Center for Chinese Medicine, The Hong Kong University of Science and Technology, Kowloon, China;* [2]*Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Kowloon, China*

WP 319 **Omni-MS: application of a one-shot multiomic data for prediction of multiple clinical biomarkers and diagnoses**; Austin Quach[1]; Alexander Yoon[1]; Whitaker Cohn[1]; Julian P Whitelegge[1]; Kym F Faull[1]; [1]*UCLA Pasarow Mass Spectrometry Laboratory, Los Angeles, CA*

WP 320 **A novel unsupervised learning approach combining protein interactions and transcriptomics to characterize the mRNA maturation machinery**; Iryna Abramchuk[1]; Karen E. Wei[2]; Lisbeth-Carolina Aguilar[2]; Alexander Ratushny[3]; Michael P. Rout[4]; John D. Aitchison[3]; Marlene Oeffinger[2]; Mathieu Lavallée-Adam[1]; [1]*University of Ottawa, Ottawa, ON;* [2]*Institut de recherches cliniques de Montréal and University of Montreal, Montreal, QC;* [3]*Seattle Biomedical Research Institute, Seattle, WA;* [4]*The Rockefeller University, New York, NY*

WP 321 **OmicLoupe: Interactive visualizations of differential expression comparisons across omics datasets**; Jakob Willforss[1]; Fredrik Levander[1]; [1]*Lund University, Department of Immunotechnology, Lund, Sweden*

**INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS
WP 322-340**

WP 322 **Data Independent Acquisition using Dual Linear Ion Trap (LIT) Miniature Mass Spectrometer**; Nan Wang[1]; Zhijun Cai[1]; Zheng Ouyang[1]; [1]*Department of Precision Instrument, Tsinghua University, Beijing, China*

WP 323 **Transportable Mass Spectrometer for Rapid Analysis of Nuclear Material and Environmental Samples**; Ankur Chaudhuri[1]; Liqian Li[1]; James Johnston[1]; Martin-Lee Cusick[1]; [1]*Canadian Nuclear Laboratories, Chalk River, ON*

WP 324 **MAss Spectrometer for Planetary EXploration – ORganic Composition Analyzer (MASPEX-ORCA) for Europa Lander**; Ryan C. Blase[1]; Chris Glein[1]; Mark Libardoni[1]; Kelly Miller[1]; Hunter Waite[1]; Gregory Miller[1]; Kate Craft[2]; Chris Bradburne[2]; Korine Ohiri[2]; Mark Perry[2]; Tessa Vanvolkenberg[2]; Katsuo Kurabayashi[3]; Xudong Fan[3]; Hongbo Zhu[3]; Anandram Venkatasubramanian[3]; Abhishek Ghosh[3]; Peter Wurz[4]; Rico Fausch[4]; [1]*Southwest*

Research Institute, San Antonio, TX; [2]Johns Hopkins University Applied Physics Laboratory, Laurel, MD; [3]University of Michigan, Ann Arbor, Michigan; [4]University of Bern, Bern, Switzerland

WP 325   **Direct on-site screening of fentanyl analogues using matrix-assisted ionization vacuum on a miniature mass spectrometer**; Xiangyu Guo[1]; Yuhan Shang[1]; Hua Bai[1]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China*

WP 326   **The effects of electrode misalignment on the performance of a linear wire ion trap**; Radhya W. Gamage[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

WP 327   **Study on the Thermal Expansion Effects of the ceramic high-resolution multiple electrodes harmonized Kingdon trap**; Anastasiia Fursova[1]; Oleg Kharybin[1]; Gleb Vladimirov[1]; Eugene (evgeny) Nikolaev[2]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

WP 328   **"Brick" Mass Spectrometer: catch up lab-scale MS and beyond**; Qian Xu[1]; Ting Jiang[1]; Zuqiang Xu[2]; Yang Tang[1]; Yanbing Zhai[1]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, China; [2]Beijing Institute of Technology, Beijing, China*

WP 329   **Characterization of Capillary Electrophoresis-Electrospray Ionization Performance of the Europan Molecular Indicators of Life Investigation (EMILI) Mass Spectrometer**; Desmond A Kaplan[1, 2]; Ryan M Danell[1, 3]; Xiang Li[1, 4]; Marco E Castillo[1]; Friso H. W. Van Amerom[1, 5]; Aaron C Noell[6]; Konstantin Zamuruyev[6]; Fernanda M Mora[6]; Peter A Willis[6]; William B Brinckerhoff[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]KapScience LLC, TEWKSBURY, MA; [3]Danell Consulting, Inc., Winterville, NC; [4]University of Maryland Balitmore, Baltimore, MD; [5]Mini-Mass Consulting Inc., Hyattsville, MD; [6]NASA Jet Propulsion Laboratory, Pasadena, CA*

WP 330   **MOMA Mass Spectrometer Laser Desorption Ionization of Mineral Samples**; Friso H.w. Van Amerom[1]; Xiang Li[2, 3]; Marco E Castillo[4]; Ryan Danell[5]; Desmond Kaplan[6]; Stephanie A Getty[3]; Andrej Grubisic[3]; William B Brinckerhoff[3]; Paul R Mahaffy[3]; Eric Lyness[7]; And The Moma Team[8]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]University of Maryland, Baltimore, Baltimore, MD; [3]NASA Goddard Space Flight Center, Greenbelt, MD; [4]ATA Aerospace, Greenbelt, MD 20770; [5]Danell Consulting, Inc., Winterville, NC; [6]KapScience LLC, TEWKSBURY, MA; [7]Microtel LLC, Greenbelt, MD, 20770; [8]Max Planck Institut für Sonnensystemforschung, Goettingen, Germany*

WP 331   **Development of MEMS-based Gas Sample Collector for a Fieldable Miniature GC-MS Instrument**; Vladimir M. Doroshenko[1]; Victor Laiko[1]; Eugene Moskovets[1]; Konstantin Novoselov[1]; Tzu-Hsuan Chang[2]; Daniel Struk[2]; Jean-Marie D. Dimandja[2]; Seung Joon Paik[2]; Milad Navaei[2]; Peter J. Hesketh[2]; *[1]MassTech, Inc., Columbia, MD; [2]Georgia Institute of Technology, Atlanta, GA*

WP 332   **Micro Ion Trap Array for Portable GC/MS Analysis of Chemical Vapors**; Michael S. Wei[1]; Ashish Chaudhary[1]; Strawn Toler[1]; R. Timothy Short[1]; Jim Alberti[1]; Ryan Bell[2]; Dustin Mcrae[1]; Matt Colvin[1]; John T Kelly[1]; *[1]SRI International, Saint Petersburg, FL; [2]Beaver Creek Analytical LLC, Lafayette, Colorado*

WP 333   **Mass Spectrometer for Planetary Exploration (MASPEX-EUROPA) a high-resolution time-of-flight mass spectrometer for NASA's Europa Clipper orbiter**; Gregory Phillip Miller[1]; Hunter Waite[2]; Tim Brockwell[2]; Paul Wilson[2]; John Hanley[2]; Ryan Blase[2]; John Roberts[2]; Keith Pickens[2]; Kelly Miller[2]; *[1]Southwest Research Institute, San Antonio, TX; [2]Southwest Research Institute (SwRI), San Antonio, TX*

WP 334   **Crude Oil Exposure of Fundulus grandis for the Quantification and Detection of Airborne Aromatic Compounds via Membrane Inlet Mass Spectrometry**; Camila Anguiano Virgen[1]; Sanjib Gurung[2]; David W. Murphy[2]; Benjamin D. Dubansky[1]; Guido F. Verbeck[1]; *[1]University of North Texas, Denton, TX; [2]University of South Florida, Tampa, FL*

WP 335   **Field Induced Fragmentation Spectra of Volatile Organic Compounds with Reactive Stage Tandem Ion Mobility Spectrometry**; Gary Eiceman[1]; Hossein Shokri[1]; Ben D Gardner[2]; *[1]New Mexico State University, Las Cruces, NM; [2]Collins Aerospace, San Diemas, CA*

WP 336   **The Characterization of Ocean Realms and Life Signatures (CORALS) Prototype**; Adrian Southard[1]; Lori Willhite[2]; Anais Bardyn[2]; Emanuel Hernandez[3]; Andrej Grubisic[3]; Ryan M. Danell[4]; Cynthia Gundersen[5]; Niko Minasola[5]; Alexander A. Makarov[6]; Christelle Briois[7]; Ricardo Arevalo[8]; *[1]Universities Space Research Association, Greenbelt, MD; [2]University of Maryland College Park, College Park, MD; [3]NASA Goddard Space Flight Center, Greenbelt, MD; [4]Danell Consulting, Inc., Winterville, NC; [5]AMU Engineering, Inc., Miami, FL; [6]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [7]CNRS UMR8038, Paris, France; [8]University of Maryland, College Park, Maryland*

WP 338   **Single particle mass spectrometry with a cycloidal mass analyzer**; Jason J Amsden[1]; Elettra Piacentino[1]; Rafael Bento Serpa[1]; Charles B. Parker[1]; Yuriy Zhilichev[2]; Roger P Sperline[3]; Robert Kingston[3]; Scott Tilden[3]; Justin Keogh[3]; Jeffrey T Glass[1]; M. Bonnner Denton[3]; *[1]Duke University, Durham; [2]Consultant, Durham, North Carolina; [3]University of Arizona, Tucson, AZ 85351*

WP 339   **Coded Aperture Imaging Comparison between Thermionic Filament and Carbon Nanotube Field Emitter Array-based Ionization Sources in a Cycloidal Mass Analyzer**; Raul Vyas[1]; Philip J. Herr[1]; Kathleen Horvath[1];

Tanouir Aloui[1]; Matthew P. Kirley[1]; Charles B. Parker[1]; Adam D. Keil[2]; James B. Carlson[3]; Justin Keogh[4]; Roger P Sperline[4]; M. Bonner Denton[4]; Brian R. Stoner[1]; Michael E. Gehm[1]; Jeffrey T Glass[1]; Jason J Amsden[1]; [1]*Duke University, Durham, NC;* [2]*Broadway Analytical, LLC, Monmouth, IL;* [3]*RTI International, Durham, NC;* [4]*University of Arizona, Tucson, AZ*

WP 340   **Title: Super-resolution in a cycloidal mass analyzer**; <u>Tanouir Aloui</u>[1]; Raul Vyas[2]; Kathleen Horvath[2]; Charles B. Parker[2]; Rafael Bento Serpa[2]; Elettra Piacentino[2]; Maria Luisa Sartorelli[3]; Jennifer Stern[4]; Justin Keogh[5]; Robert Kingston[5]; Scott Tilden[5]; Roger P Sperline[5]; M. Bonner Denton[5]; Michael E. Gehm[2]; Jeffrey T Glass[2]; Jason J Amsden[2]; [1]*Duke University, Durham, NC;* [2]*Pratt School of Engineering, Duke University, Durham, NC;* [3]*Universidade Federal de Santa Catarina, Trindade, Brazil;* [4]*NASA Goddard Space Flight Center, Greenbelt, MD;* [5]*Department of Chemistry and Biochemistry University of Arizona, Tucson, AZ85721*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING II
WP 341-360

WP 341   **Combined Atomic and Molecular (CAM) Ionization: The Diversity of the Liquid Sampling–Atmospheric Pressure Glow Discharge on a Compact Mass Spectrometer**; <u>Tyler J. Williams</u>[1]; R. Kenneth Marcus[1]; Jacob R. Bills[1]; Jamey Jones[2]; [1]*Clemson University, Clemson, SC;* [2]*Advion, Ithaca, NY*

WP 342   **Detection of Perfluoroalkyl and Polyfluoroalkyl Substances through Automation of ASAP**; <u>Frank S. Yenchick</u>[1]; Long Luo[1]; Sarah Trimpin[1]; [1]*Wayne State University, Detroit, MI*

WP 343   **Mechanism of Ionization Suppression from Ion Evaporation Model and a System for Real-Time Correction for Biological Samples**; <u>Thomas R Covey</u>[1]; Andries P Bruins[2]; Chang Liu[1]; [1]*SCIEX, Concord, ON;* [2]*University of Groningen, Groningen, Netherlands*

WP 344   **Efficient introduction of ionic compounds into LC-MS using the improved ESI unit; Application to dirty samples**; <u>Takanari Hattori</u>[1]; Miho Kawashima[1]; Wataru Fukui[1]; Kazuo Mukaibatake[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

WP 345   **Computer Assisted Development of 3D Printed Analytical Devices for Customized Open Port Probe-Electrospray Mass Spectrometry**; <u>Piotr Sosnowski</u>[1]; Gérard Hopfgartner[1]; [1]*Life Sciences Mass Spectrometry, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland*

WP 346   **Enhanced Analysis of Polymers with an Inductively-heated Impactor Spray Source**; <u>Steve Bajic</u>[1]; Claudie Black[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

WP 347   **Ion Dynamics Simulation Framework (IDSimF): An Open Source Trajectory Simulation Framework**; <u>Walter Wissdorf</u>[1]; Duygu Erdogdu[1]; Marco Thinius[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany*

WP 348   **MALDI-2 laser post-ionization on a trapped ion mobility orthogonal time of flight instrument**; <u>Simeon Vens-Cappell</u>[1]; Henning Peise[1]; Andreas Haase[1]; Annika Koch[1]; Jens Hoehndorf[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany*

WP 349   **Transport of Plasma generated Ions into a Fourier Transform Quadrupole Ion Trap using viscous gas flows**; <u>Chris Vico Heintz</u>[1]; Yessica Brachthäuser[2]; Hendrik Kersten[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany;* [2]*INFICON GmbH, Cologne, Germany*

WP 350   **High Sensitivity Analysis of Steroid Hormones with modified ESI to improve desolvation efficiency**; <u>Yuki Uno</u>[1]; Yohei Toji[1]; Yusuke Inohana[1]; Tomoya Kudo[1]; Kazuo Mukaibatake[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

WP 351   **Real Time Continuous Monitoring of Nucleophilic Acyl Substitution and 1,4-Nucleophilic Addition Reactions under Positive-ion Helium-Plasma Ionization (HePI) Mass Spectrometric Conditions**; Athula B. Attygalle[1]; <u>Ramu Errabelli</u>[2]; Julius Pavlov[1]; Isra Hassan[1]; Zhaoyu Zheng[1]; David Douce[3]; Steve Bajic[3]; [1]*Stevens Institute of Technology, Hoboken, NJ;* [2]*Stevens Institute of Technology, Jersey City, NJ;* [3]*Waters Corporation, Wilmslow, United Kingdom*

WP 352   **Hydrogen plasma based chemical ionization source for GC-MS**; <u>Steffen Bräkling</u>[1]; Kai Kroll[1]; Hendrik Kersten[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany*

WP 353   **On-line process monitoring of complex gas mixtures using a novel combination of oa-ToF systems with pulsed soft photoionization sources**; Sven Ehlert[1, 2]; Jan Heide[2]; <u>Andreas Walte</u>[1]; Ralf Zimmermann[2, 3]; [1]*Photonion GmbH, Schwerin, Germany;* [2]*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany;* [3]*Heltmholtz Center, Munich, Germany*

WP 354   **Rapid polyaromatic hydrocarbon measurement in soils with isomer differentiation: Condensed Phase Membrane Introduction Mass Spectrometry with in situ Chemical Ionization**; <u>Gregory W. Vandergrift</u>[1, 2]; Erik T. Krogh[1, 2]; Christopher G. Gill[1, 2, 3, 4]; [1]*Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC;* [2]*University of Victoria, Victoria, British Columbia;* [3]*Simon Fraser University, Burnaby, BC;* [4]*University of Washington, Seattle, WA*

WP 355 **Acoustic Ejection Full Scan MS Analysis in Support of High Throughput Compound Plate QC**; Jun Zhang[1]; Yong Zhang[1]; Chang Liu[2]; Tom Covey[2]; Shu Li[1]; Harold Weller[1]; Wilson Shou[1]; *[1]Bristol-Myers Squibb, Lawrenceville, NJ; [2]SCIEX, Concord, ON*

WP 356 **Development of High-Performance Capillary Vibrating Sharp-edge Spray Ionization (cVSSI) for Mass Spectrometry Analysis**; Chong Li[1]; Kushani Attanayake[1]; Stephen J. Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

WP 357 **Native MS studies of proteins using capillary Vibrating Sharp-edge Spray Ionization (cVSSI)**; Daud Sharif[1]; Samira Hajian Foroushani[1]; Kushani Attanayake[1]; Anthony Debastiani[1]; Chong Li[1]; Peng Li[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

WP 358 **Factors affecting ionization of small molecules by capillary vibrating sharp-edge spray ionization (cVSSI)**; Kinkini Udara Jayasundara[1]; Anthony Debastiani[1]; Chong Li[1]; Daud Sharif[1]; Sara Macios[1]; Peng Li[1]; Stephen J Valentine[1]; *[1]West Virginia University, Morgantown, WV*

WP 359 **Velox Sample Cartridge with Snap-in Solid-Phase Extraction Column for Paper Spray Mass Spectrometry**; Chau Nguyen[1]; Nicholas Manicke[2]; *[1]indiana University - Purdue University Indianapolis, Indianapolis, IN; [2]Indiana University - Purdue University Indianapolis, Indianapolis, IN*

WP 360 **Advances in Automated Multi-ionization Mass Spectrometry: ESI, SAI, MAI**; Khoa Hoang[1]; Milan Pophristic[1]; Sarah Trimpin[1, 2]; Charles N Mcewen[1, 3]; *[1]MSTM LLC, Newark, DE; [2]Wayne State University, Detroit, MI; [3]University of the Sciences in Philadelphia, Philadelphia, Pennsylvania*

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WP 361 **Ion/Ion Proton Transfer Reaction for Enhancing Peak Capacity in an Ion Mobility/Mass Spectrometry Bottom-up Proteomics Experiment**; Rebecca L Cain[1]; Ian Webb[2]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN; [2]Indiana University - Purdue University Indianapolis, Indianapolis, IN*

WP 362 **Rapid Characterization of Drug Conjugation in a Monoclonal Antibody by High-Resolution Ion Mobility Separations in Structures for Lossless Ion Manipulations**; Gabe Nagy[1]; Isaac K. Attah[1]; Christopher R. Conant[1]; Weijing Liu[1]; Sandilya V. B. Garimella[1]; Harsha P. Gunawardena[2]; Jared B. Shaw[1]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Johnson and Johnson, Spring House, PA*

WP 363 **Utilizing Ion Mobility Workflows for Rapid Metabolomics Combined with Collisional Cross Sectional (CCS) Libraries for Increased Specificity**; Adam M King[1, 2]; Mark Ritchie[3]; Lee Gethings[1]; Lauren Mullin[4]; Robert Plumb[4]; Ian D Wilson[5]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Murdoch University, Perth, Australia; [3]Waters Pacific Pte. Ltd., Singapore, Singapore; [4]Waters Corporation, Milford, MA; [5]Imperial College London, London, United Kingdom*

WP 364 **High Throughput Analysis of Antidepressant Drugs in Human Plasma Sample by Liquid Chromatography Vacuum Differential Mobility Spectrometry-Mass Spectrometry**; Maria Fernanda Cifuentes Girard[1]; Patrick Knight[2]; Roger Giles[2]; Gérard Hopfgartner[1]; *[1]Life Sciences Mass Spectrometry, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; [2]Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom*

WP 365 **Application of Ion Mobility Specificity to Investigate Food Additive Charged Isomers and Conformers**; Michael Mccullagh[1]; Severine Goscinny[2]; Kenneth Rosnack[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Sciensano, Brussels, Belgium; [3]Waters Corporation, Milford, MA*

WP 366 **Structures for Lossless Ion Manipulation-MS for High Resolution, High Throughput Lipid Biomarker Analysis**; Kelly Wormwood[1]; Ravinder Earla[1]; James R. Arndt[1]; Liulin Deng[1]; Anisha Yadav[1]; Stephen Krufka[1]; Daniel Debord[1]; Laura Maxon[1]; Kim Ekroos[2]; *[1]MOBILion Systems Inc., Chadds Ford, PA; [2]Lipidomics Consulting Ltd, Esbo, Finland*

WP 367 **Profiling the Indole Alkaloids in Yohimbe Bark with UPLC and High Resolution Ion Mobility Spectrometry Coupled with Mass Spectrometry**; Andrew Baker[1]; Pei Chen[2]; Jianghao Sun[3]; *[1]Waters, Inc., Pleasanton, CA; [2]USDA-ARS, Beltsivlle, MD; [3]USDA-ARS, Beltsville, MD*

WP 368 **DMS-MS for Rapid Characterization of Polysorbate 80 Samples**; Jay S Bhanot[1]; Nan Wang[1]; Alice Newman[2]; Bangping Xiang[2]; Li-Kang Zhang[2]; Kudrat Goswami[2]; Damon Barbacci[2]; Simon Hamilton[2]; Scott A. Mcluckey[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co., Kenilworth, NJ*

WP 369 **Identification of Structural Isomers Utilizing a Deep Neural Network with a Metabolite-Specific Compound Library**; Maria V. Fawaz[1]; Ian S. Mcintosh[1]; Xiang Yu[1]; Richard Gundersdorf[1]; Mark T. Cancilla[1]; *[1]Merck, West Point*

WP 370 **Utilizing Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry (LC-IMS-MS) to Assess INLIGHT™ Derivatized N-linked Glycans in Biological Samples**; Karen E. Butler[1]; Jaclyn Gowen

Kalmar[1]; Brendan X. Maclean[2]; Thomas J. Montine[3]; Michael J. MacCoss[2]; David C. Muddiman[1]; Erin S. Baker[1]; [1]*Department of Chemistry, North Carolina State University, Raleigh, NC;* [2]*Department of Genome Sciences, University of Washington School of Medicine, Seattle, WA;* [3]*Department of Pathology, Stanford University, Stanford, CA*

WP 371   **Deeper proteome coverage of musculoskeletal samples**; Emma Doud[1]; Xiaoling Zhong[1]; Joseph Rupert[1]; Matt Willetts[2]; Shourjo Ghose[2]; Teresa Zimmers[1, 3]; Amber L Mosley[1]; [1]*Indiana University School of Medicine, Indianapolis, IN;* [2]*Bruker Scientific LLC, Billerica, MA;* [3]*Richard L. Rhoudebush VA Medical Center, Indianapolis, IN*

WP 372   **Cyclic Ion Mobility (cIM) combined with ECD MS/MS for characterization and sequencing of isomeric proteoforms**; Frederik H. V. Holck[1]; Dale A. Cooper-Shepherd[2]; Pavel V. Shliaha[1]; James I. Langridge[2]; Ole N. Jensen[1]; [1]*University of Southern Denmark, Odense M, Denmark;* [2]*Waters Corporation, Wilmslow, United Kingdom*

WP 373   **The Application of Ion Mobility-Mass Spectrometry towards Structural Characterization of α-Synuclein**; John M. Gordon[1]; Christopher S. Mallis[1]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX*

WP 374   **Towards native top-down sequence analysis of protein isomers using tandem-trapped ion mobility spectrometry / mass spectrometry (Tandem-TIMS/MS)**; Kirsten Tucker[1]; Mengqi Chai[1]; Fanny C Liu[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

WP 375   **Using SLIM-based ion mobility with on-board CID together with cryogenic ion spectroscopy for glycan analysis**; Priyanka Bansal[1]; Robert P Pellegrinelli[1]; Vasyl Yatsyna[1]; Ali Abi Khodr[1]; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Eduardo Carrascosa[1]; Lei Yue[1]; Natalia Yalovenko[1]; Vicki H. Wysocki[2]; Thomas R. Rizzo[1]; [1]*Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland;* [2]*The Ohio State University, Columbus, OH*

WP 376   **PASEF-DDA enables deep coverage single-shot phosphoproteomics and ion mobility-based elucidation of phosphosite isomers**; Thomas Michna[1]; Mateusz Krzysztof Lacki[1]; Ute Distler[1]; Stephanie Kaspar-Schoenefeld[2]; Scarlet Koch[2]; Nadine Vewinger[1]; Claudia Paret[1]; Alex Henneman[3]; Joerg Faber[1]; Connie R. Jimenez[3]; Stefan Tenzer[1]; [1]*Medical Center of the Johannes Gutenberg University, Mainz, Germany;* [2]*Bruker Daltonic GmbH, Bremen, Germany;* [3]*Amsterdam UMC, Amsterdam, Netherlands*

WP 377   **Ion Mobility Mass Spectrometry as an Efficient Tool for Identification of Streptorubin B in Streptomyces coelicolor M145**; Andrew P Marshall[1]; Andrew R Johnson[2]; Marvin M Vega[3]; Regan J Thomson[4]; Erin E Carlson[5]; [1]*University of Minnesota, Minneapolis, MN;* [2]*Indiana University, Bloomington, IN;* [3]*Northwestern University, Evanston, IL;* [4]*Northwestern University, Evanston, IL/60208;* [5]*University of Minnesota, Minneapolis, MN/55455*

WP 378   **At-line profiling degradation products of peptide drug teriparatide by advanced robotics coupled with ion mobility mass spectrometry: A top-down approach**; Mack Shih[1]; Maxwell Korang-Yeboah[1]; Muhammad Ashraf[1]; Sau Lee[1]; Patrick Faustino[1]; Jinhui Zhang[1]; [1]*FDA, Silver Spring, MD*

WP 379   **Advancing Data Independent Acquisition and Data Processing Strategies for IM-QTOFMS**; Max L. Feuerstein[1]; Ruwan T. Kurulugama[2]; Hiroshi Tsugawa[3, 4]; Tim Causon[1]; Stephan Hann[1]; [1]*University of Natural Resources and Life Sciences (BOKU), Vienna, Austria;* [2]*Agilent Technologies, Santa Clara, CA;* [3]*RIKEN Center for Sustainable Resource Science, Yokohama, Japan;* [4]*RIKEN Center for Integrative Medical Sciences, Yokohama, Japan*

WP 380   **Trapped ion mobility ultra-high resolution mass spectrometry for deciphering complex petroleomic mixtures — Insights into compositional space and isomeric diversity**; Carlos Afonso[1, 2]; Christopher Rüger[3]; Johann Le Maître[2, 4, 5]; Mark E. Ridgeway[6]; Christopher Thompson[6]; Melvin A. Park[6]; Pierre Giusti[5, 7]; [1]*University of Rouen-Normandy, Mont Saint Aignan, France;* [2]*International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France;* [3]*Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany;* [4]*University of Rouen-Normandy, Mont-Saint-Aignan, France;* [5]*Total Refining and Chemicals, Harfleur, France;* [6]*Bruker Daltonics, Billerica, MA;* [7]*International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France*

WP 381   **Paper Spray Ionization-Ion Mobility Mass Spectrometry (PSI-IM MS) Direct from Skin Swabs for Rapid Diagnosis of Parkinson's Disease**; Depanjan Sarkar[1]; Drupad K Trivedi[1]; Eleanor Sinclair[1]; Sze Hway Lim[1]; Caitlin Walton-Doyle[1]; Kaneez Jafri[1]; Joy Milne[1]; Monty Silverdale[1]; Perdita E Barran[1]; [1]*University of Manchester, Manchester, United Kingdom*

WP 382   **Rapid Chemical Description of Organic Aerosols with a Direct Inlet Probe Coupled to Trapped Ion Mobility Time-of-Flight Mass Spectrometry**; Lukas Friederici[1]; Christopher Paul Rüger[2]; Janne Jänis[3]; Christian Albers[4]; Heino M. Heyman[5]; Ralf Zimmermann[2, 6]; [1]*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany;* [2]*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany;* [3]*University of Eastern Finland, Joensuu, Finland;* [4]*Bruker Daltonik GmbH, Bremen, Germany;* [5]*Bruker Scientific LLC, Billerica, MA;* [6]*Helmholtz Zentrum München German Research Center for Environmental Health, Cooperation Group of Comprehensive Molecular Analytics, München, Germany*

WP 385   **The Identification of Intact Phase II Steroid Metabolites in Human Urine Utilizing Liquid Chromatography-Ion Mobility-Mass Spectrometry**; Don E. Davis, Jr. [1]; Gustavo de Albuquerque Cavalcanti[2]; Monica C. Padilha[2]; Katrina L. Leaptrot[1]; Nadjali A. Chung[1]; Jody C. May[1]; John A. McLean[1]; Henrique M.g. Pereira[2]; [1]*Department of*

Chemistry, Center for Innovative Technology, Vanderbilt Institute of Chemical Biology, Vanderbilt Institute for Integrative Biosystems Research and Education, Vanderbilt–Ingram Cancer Center, Vanderbilt University, Nashville, TN; [2]Brazilian Doping Control – LBCD – Chemistry Institute – Federal University of Rio de Janeiro,, Rio de Janeiro, Brazil

WP 386   **Multiplexed IR spectroscopy of ion-mobility separated glycans using Hadamard transform**; Vasyl Yatsyna[1,2]; Ali H Abikhodr[1]; Thomas R. Rizzo[1]; *[1]EPFL/LCPM, Lausanne, Switzerland; [2]University of Gothenburg, Gothenburg, Sweden*

WP 387   **The Paternò-Büchi Reaction as a Method for Improved Ion Mobility Separation of Isomeric Steroids**; Stine S. H. Olsen[1]; Samuel W Maddox[1]; Diane C Velosa[1]; Aurora Burkus-Matesevac; Christopher D. Chouinard[1]; *[1]Florida Institute of Technology, Melbourne, FL*

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WP 388 **10 min LC-MSMS analysis of fatty acids in triacylglycerols to compare human serum and food**; Doriane Toinon[1]; Yamada Masaki[1]; [1]*Shimadzu corporation, Kyoto, Japan*

WP 389 **Systematic Approach to Method Development for Lipidomics Analysis of Biological Samples Using Trend Analysis and Lipostar**; Rachelle Golden[1]; Laura Goracci[2]; Paolo Tiberi[3]; Gabriele Cruciani[2]; Lilu Guo[1]; Alla Kloss[1]; [1]*Sanofi, Vitry Sur Seine, France; [2]University of Perugia, Perugia, Italy; [3]Molecular Discovery, Ltd., Borehamwood, United Kingdom*

WP 390 **Analysis and Characterization of Glycolipids in Human and Bovine Milk**; Abby S. Gelb[1]; Silvia Ringler[2]; Bernd Stahl[1, 2, 3]; Catherine E. Costello[1]; [1]*Boston University School of Medicine, Boston, MA; [2]Danone Nutricia Research, Utrecht, Netherlands; [3]Utrecht University, Utrecht, Netherlands*

WP 391 **Untargeted lipidomic analysis of human retinas using LC-MS/MS and MALDI imaging mass spectrometry**; Ankita Kotnala[1, 2]; David M Anderson[1]; Jarod A. Fincher[1]; Nathan Heath Patterson[1]; Lee S Cantrell[1]; Jeffrey D. Messinger[2]; Christine A. Curcio[2]; Kevin L. Schey[1]; [1]*Department of Biochemistry, Vanderbilt University, Nashville, TN; [2]Department of Ophthalmology and Visual Sciences, University of Alabama at Birmingham, Birmingham, AL*

WP 392 **From plants to ants: Spatiotemporal mapping of lipidomic changes in the leaf-cutter ant fungal garden ecosystem during plant degradation**; Lily Khadempour[1]; Jennifer E. Kyle[2]; Bobbie-jo M. Webb-robertson[2]; Carrie D. Nicora[2]; Richard D. Smith[2]; Mary S. Lipton[2]; Cameron R. Currie[1]; Erin S. Baker[3]; Kristin E. Burnum-Johnson[2]; [1]*University of Wisconsin-Madison, Madison, WI; [2]Pacific Northwest National Laboratory, Richland, WA; [3]North Carolina State University, Raleigh, NC*

WP 393 **In-depth high throughput triacylglyceride profiling with three fatty acids chains information using a modified MRM3 method**; Matias E Cabruja[1]; Mathew C Ellenberger[1]; Kevin Contrepois[1]; Michael P Snyder[1]; [1]*Stanford University, Stanford, CA*

WP 394 **BIOANALYSIS OF LIPIDS: COMPARISON BETWEEN DIRECT INFUSION WITH DIFFERENTIAL ION MOBILITY AND REVERSE-PHASE ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY METHODS**; Zhengzheng Zhang[1]; Nelus Schoeman[1]; Isabelle Kohler[1]; Amy Harms[1]; Peter Lindenburg[1, 2]; Thomas Hankemeier[1]; [1]*Leiden university, leiden, Netherlands; [2]Hogeschool Leiden, Leiden, Netherlands*

WP 395 **Serum lipid profiling from a randomized trial on the effects of dietary patterns on obesity**; Sunhee Jung[1]; Ji-Hee Shin[2]; Seoyoung Jang[1, 3]; Dong-Mi Shin[4]; Geum-Sook Hwang[1, 3]; [1]*Korea Basic Science Institute, Seoul, South Korea; [2]Seoul National University, Seoul, South Korea; [3]Ewha Womans University, Seoul, South Korea; [4]Seoul Naional University, Seoul, South Korea*

WP 396 **High Resolution Accurate Mass Spectrometry of Intact Lipopolysaccharides from Enteric Bacteria Carrying O-specific Polysaccharides**; Elder Pupo[1]; Peter Van Der Ley[1]; Hugo D. Meiring[1]; [1]*Institute for Translational Vaccinology, Bilthoven, Netherlands*

WP 397 **Lithium ion adduction-based UPLC-MS/MS analysis of multi-class ketolic steroid hormones containing a 3-hydroxyl group**; Qiuyi Wang[1]; Kimiko Shimizu[2]; Kanako Maehata[2]; Yue Pan[1]; Koki Sakurai[1]; Takatoshi Hikida[1]; Yoshitaka Fukada[2]; Toshifumi Takao[1]; [1]*Osaka University, Suita, Japan; [2]The University of Tokyo, Tokyo, Japan*

WP 398 **In vivo real-time SpiderMass™ analysis for dermatology and cosmetics assessment**; Philippe Saudemont[1, 2]; Michel Salzet[1]; Gwendal Josse[2]; Isabelle Fournier[1]; [1]*University of Lille, Villeneuve d'Ascq, France; [2]Pierre Fabre DermoCosmetic, Toulouse, France*

WP 399 **Oncofinder: a novel platform for screening benignant nevi from melanomas based on lipid phenotype using mass spectrometry and machine learning**; Roberto A. Fernández Regueira[1]; Egoitz Astigarraga[1]; José A. Fernández[2]; Dolores Boyano[2]; Aintzane Asurmendi[2]; Michael N. Nairn[3]; Shaukat Ibrahim[3]; Simona Salivo[3]; Matthew E. Openshaw[3]; Gabriel Barreda-Gómez[1]; [1]*IMG Pharma Biotech S.L., Derio, Spain; [2]University of the Basque Country (UPV/EHU), Barrio Sarriena, Spain; [3]Shimadzu, Manchester, United Kingdom*

WP 400 **AMP-activated protein kinase activation inhibits ferroptosis through PUFA metabolism**; Fereshteh Zandkarimi[1]; Hyemin Lee[2]; Boyi Gan[2]; Brent R. Stockwell[1]; [1]*Columbia University, New York, NY; [2]University of Texas MD Anderson Cancer Center, Houston, TX*

WP 401 **Infusion MS/MSALL with Differential Mobility Separation : A High-throughput Lipidomic Solution for Untargeted Profiling** ; Mackenzie Pearson[1]; Paul Norris[2]; Santosh Kapil[2]; Darren Dumlao[3]; [1]*Sciex, Redwood City, CA; [2]Sciex, Framingham, MA; [3]SCIEX, Redwood Shores, California 1201*

WP 403 **Hight throughput lipidomics for bacterial phenotyping**; Rutan Zhang[1]; Nate K. Ashford[2]; Amy Li[2]; Dylan H. Ross[2]; Brian J. Werth[2]; Libin Xu[2]; [1]*University of Washington, seattle, WA; [2]University of Washington, Seattle, WA*

WP 404 **Analysis of Stable Isotope Labeled N-docosahexaenoylphosphatidylethanolamine Molecular Species Distribution in Neuronal Cell Culture**; Karl R Kevala[1]; Michel Lagarde[2]; Arthur Spector[1]; Hee-Yong Kim[1]; *[1]National Institutes of Health, Rockville, MD; [2]Universite de Lyon, Lyon, France*

WP 405 **Non-targeted Lipidomic Analysis Paired with Semi-targeted Profiling of 3-Picolylamide Fatty Acid Derivatives for the Characterization of Microbiome Samples**; Lucas Veillon[1]; Marc Warmoes[1]; Abdul Wadud Khan[1]; Reetakshi Arora[1]; Jennifer Wargo[1]; John N Weinstein[1]; Philip L Lorenzi[1]; *[1]MD Anderson Cancer Center, Houston, TX*

WP 407 **Alterations in mouse brain lipidome during neurodevelopment and in a model of Smith-Lemli-Opitz syndrome**; Amy Li[1]; Kelly M Hines[1, 2]; Libin Xu[1]; *[1]University of Washington, Seattle, WA; [2]University of Georgia, Athens, GA*

WP 408 **Lipidomic analysis of plasma from patients with cervical cancer and cervical intraepithelial neoplasia using LC-MS approach**; Seoyoung Jang[1]; Miso Nam[1]; Sunhee Jung[1]; Mi Kyung Kim[2]; Geum-Sook Hwang[1]; *[1]Korea Basic Science Institute, Seoul, South Korea; [2]National Cancer Center, Goyang-si, South Korea*

WP 409 **Untargeted lipidomics of viral particles and cell lysates following vesicular stomatitis virus infection**; Katherine E. Havranek[1]; Melinda A. Brindley[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

WP 410 **Unequivocal mapping of ether lipids by LC-MS/MS by using plasmalogen-deficient mouse tissues**; Jakob Koch[1]; Katharina Lackner[2]; Yvonne Wohlfarter[1]; Sabrina Sailer[2]; Johannes Zschocke[1]; Katrin Watschinger[2]; Markus Keller[1]; *[1]Institute of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; [2]Institute of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria*

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WP 412 **Effect of therapeutic agent BS11 on interaction betweenmetabolic responses and intestinal microbes of metabolic diseases**; Jung-Eun Lee[1]; Jeeyoun Jung[1]; *[1]Korea Institute of Oriental Medicine, Daejeon, South Korea*

WP 413 **Characterization of Rare X-Chromosome Deletion Disorders Using Metabolomics and Lipidomics Workflows by High-Resolution Mass Spectrometry**; Hoda Safari Yazd[1]; Vanessa Y. Rubio[1]; Richard A. Yost[1]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL*

WP 414 **Development of a Novel Metabolomics Workflow using 95% 13C Internal Standard with Liquid Chromatography and Ion Mobility-Mass Spectrometry**; Robin H.J. Kemperman[1]; Chris W.W. Beecher[2]; Timothy J. Garrett[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL; [2]IROA Technologies, Chapel Hill, NC*

WP 415 **Strong sexual dimorphism of plasma metabolites in 30 gene knockout mice strains by multi-platform mass spectrometry analyses**; Ying Zhang[1, 2]; Dinesh K. Barupal[1]; Sili Fan[1]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, UC Davis, Davis, CA; [2]Department of Chemistry, University of California, Davis, Davis, CA*

WP 416 **Inter-laboratory comparison of metabolite measurements for metabolomics data integration**; Yoshihiro Izumi[1]; Fumio Matsuda[2]; Akiyoshi Hirayama[3]; Kazutaka Ikeda[4]; Yoshihiro Kita[5]; Kanta Horie[6]; Daisuke Saigusa[7]; Kosuke Saito[8]; Yuji Sawada[9]; Hiroki Nakanishi[10]; Nobuyuki Okahashi[2]; Masatomo Takahashi[1]; Motonao Nakao[1]; Kosuke Hata[1]; Yutaro Hoshi[11]; Motohiko Morihara[12]; Kazuhiro Tanabe[13]; Takeshi Bamba[1]; Yoshiya Oda[5]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Graduate School of Information Science and Technology, Osaka University, Osaka, Japan; [3]Institute for Advanced Biosciences, Keio University, Yamagata, Japan; [4]Kazusa DNA Research Institute, Chiba, Japan; [5]Graduate School of Medicine, The University of Tokyo, Tokyo, Japan; [6]Translational Science, Neurology Business Group, Eisai Co., Ltd., Ibaraki, Japan; [7]Tohoku Medical Megabank Organization, Tohoku University, Miyagi, Japan; [8]Division of Medical Safety Science, National Institute of Health Science, Kanagawa, Japan; [9]RIKEN Center for Sustainable Resource Science, Kanagawa, Japan; [10]Research Center for Biosignal, Akita University, Akita, Japan; [11]Pharmacokinetic Research Laboratories, Ono Pharmaceutical Co., Ltd., Ibaraki, Japan; [12]Translational Research Laboratories, Ono Pharmaceutical Co., Ltd., Osaka, Japan; [13]Medical Solution Segment, LSI Medience Corporation, Tokyo, Japan*

WP 417 **Developing an Integrated Metabolomics Workflow: From High Resolution MS Data to Biochemical Pathway Mapping Using Targeted and Untargeted Approaches**; Richard Schneider[1]; John Janiszewski[1]; Sam Michael[1]; Matt Hall[1]; Stephen Ferguson[1]; Michael Iannotti[1]; Surbhi Poddar[2]; Maheswari Karthikeyan[2]; Sunil Dhakad[2]; Raghav Sehgal[3]; Rebecca Cardone[3]; Qiushi Sun[3]; Richard G. Kibbey[3]; *[1]NCATS/NIH, Rockville, MD; [2]Elucidata, Delhi, India; [3]Yale University, New Haven, CT*

WP 418 **Untargeted FTICR-MS Based Plasma Metabolomic Analysis and Translation to Type 2 Diabetes**; Yanlong Zhu[1]; Benjamin Wancewicz[1]; Michael Schaid[1]; Kent Wenger[1]; Yutong Jin[1]; Heino M. Heyman[2]; Christopher Thompson[2]; Aiko Barsch[3]; Allan R Brasier[1]; Michelle Kimple[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin; [2]Bruker Daltonics, Billerica, MA; [3]Bruker Daltonics, Bremen, Germany*

WP 419   **A single LC-UV/RI-MS/MS configuration for metabolomics and exometabolomics approaches to explore metabolic network operation of Ustilago trichophora**; An N. T. Phan[1]; Lars M. Blank[1]; [1]*RWTH Aachen University, iAMB - Institute of Applied Microbiology, ABBt – Aachen Biology and Biotechnology, Aachen, Germany*

WP 420   **Liquid Chromatography Tandem Mass Spectrometric Analysis of Tryptophan-Kynurenine Catabolism in Biological Samples**; Jaeman Byun[1]; Subramaniam Pennathur[2]; Anna Mathew[3]; [1]*University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan; [3]University of Michiagan, Ann Arbor, MI*

WP 421   **High Performance Chemical Isotope Labeling (HP-CIL) LC-MS Platform for High-Coverage Quantitative Metabolomics**; Shuang Zhao[1, 2]; Liang Li[1]; [1]*University of Alberta, Edmonton, AB; [2]Nova Medical Testing Inc., Edmonton, AB*

WP 422   **Comprehensive metabolomics of wine using LC-QTOFMS and LC-TQMS; Novel workflow to transfer analytical method from LC-QTOFMS to LC-TQMS**; Tetsuo Iida[1]; Akane Murayama[2]; Takanari Hattori[2]; Jun Watanabe[2]; [1]*Shimadzu Corporation, Global Application Development Center, Kyoto, Japan; [2]Shimadzu Corporation, MS Business Unit, Kyoto, Japan*

WP 423   **Single egg metabolomics as the latest tool in the Drosophila Melanogaster toolbox**; Ryan D Sheldon[1]; Eduardo Perez-Mojica[1]; Ellen Griggs[1]; Christine Isaguirre[1]; Abigail Ellis[1]; Brejnev M. Muhire[1]; Russel G. Jones[1]; Adelheid Lempradl[1]; [1]*Metabolic and Nutritional Programming, Center for Cancer and Cell Biology, Van Andel Institute, Grand Rapids, MI*

WP 424   **Liquid chromatography-tandem mass spectrometry-based metabolite profiling in the hearts of germ-free and conventionalized mice**; Chaoyi Wu[1, 2]; Kazuyuki Kasahara[3]; Federico Rey[3]; Laura-Isobel Mccall[2, 4, 5]; [1]*University of Oklahoma, Dept. of Chem & Biochem, Norman, Oklahoma; [2]Laboratories of Molecular Anthropology and Microbiome Research, University of Oklahoma, Norman, OK; [3]Department of Bacteriology University of Wisconsin-Madison, Madison, Wisconsin; [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; [5]Department of Microbiology and Plant Biology, University of Oklahoma, Norman, OK*

WP 425   **Maximizing High Confidence Compound Identification by An Improved LC-MS Workflow for Antibody Process Development**; Jikang Wu[1]; Hongxia Wang[1]; Xueqing Zhao[1]; Haibo Qiu[1]; Ning Li[1]; [1]*Regeneron Pharmaceuticals Inc., Tarrytown, NY*

WP 426   **Metabolic rewiring of cardiomyocytes after acute infection of Trypanosoma cruzi**; Gabriela Venturini[1, 2]; Juliana Alvim[2]; Kallyandra Padilha[2]; Karina Cardozo[3]; Valdemir Carvalho[3]; Jose Eduardo Krieger[2]; Jonathan Seidman[1]; Christine Seidman[1, 4]; Alexandre Pereira[1, 2]; [1]*Harvard Medical School, Boston, MA; [2]Heart Institute, Medical School, USP, Sao Paulo, Brazil; [3]Fleury Group, Sao Paulo, Brazil; [4]Brigham and Women's Hospital, Boston, MA*

WP 427   **Elucidating unknown pathways in Plasmodium falciparumwith labeled metabolomics**; Conor Jenkins[1, 2]; Ioanna Ntai[3]; Amanda Souza[3]; Benjamin Orsburn[2, 4]; [1]*Hood College, Frederick, MD; [2]Proteomic Und Genomic Sciences, Glen Rock, PA; [3]Thermo Fisher Scientific, San Jose, California; [4]University of Virginia School of Medicine, Charlottesville, VA*

METABOLOMICS: UNTARGETED METABOLITE PROFILING I
WP 428-448

WP 428   **Studying Neural Tissue Formation by Analyzing Neural-Tissue Fated Cell Clones from Developing X. laevis Embryos using LC-HRMS**; Jie Li[1]; Peter Nemes[1]; [1]*University of Maryland College Park, College Park, MD*

WP 429   **+++-*AA systematic approach to transform untargeted profiling to pseudo-targeted analysis for metabolomics study based on liquid chromatography mass spectrometry**; Ziquan Fan[1]; Niusheng Xu[1]; [1]*Thermo Fisher Scientific, Shanghai, China*

WP 430   **Elucidation of carotenoids in microalgae formulations by ultra-high resolution mass spectrometry combined with APCI**; Eduardo Sommella[1]; Emanuela Salviati[1]; Giulio Maria Conte[1]; Matthias Witt[2]; Pietro Campiglia[1]; [1]*University of Salerno, Fisciano, Italy; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 431   **Metabolic changes in murine hair follicles treated with Procyanidine-B2 rich nutraceuticals studied by Magnetic Resonance Mass Spectrometry (MRMS)**; Eduardo Sommella[1]; Emanuela Salviati[1]; Matthias Witt[2]; Christopher Thompson[3]; Pietro Campiglia[1]; [1]*University of Salerno, Fisciano, Italy; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

WP 432   **UNTARGETED LIPIDOMICS ANALYSIS OF PLASMA SAMPLES FROM DYSLIPIDEMIC PATIENTS**; Anna Maria Alves De Piloto Fernandes[1]; Gustavo Henrique Bueno Duarte[2]; Alex Aparecido Rosini Silva[1]; Joyce Aparecida Barreto[3]; Márcia Aparecida Antonio[3]; Andréia de Melo Porcari[1]; Patricia de Oliveira Carvalho[1]; [1]*Universidade São Francisco, Bragança Paulista, Brazil; [2]Universidade Estadual de Campinas, Campinas, Brazil; [3]Unidade Integrada de Farmacologia e Gastroenterologia, Bragança Paulista, Brazil*

WP 434   **Proteometabolomics identifies modulated purine metabolism as a mechanism of melphalan resistance in multiple myeloma**; David C. Koomen[1, 2]; Mark B. Meads[1]; Dario M. Magaletti[1]; Joy D. Guingab-Cagmat[3]; Paula S.

Oliveira[1]; Bin Fang[1]; Min Liu[1]; Victoria Izumi[1]; Laurel E. Meke[3]; Eric A. Welsh[1]; Steven A. Eschrich[1]; Timothy J. Garrett[3]; John M. Koomen[1]; Kenneth H. Shain[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL; [2]University of South Florida, Tampa, FL; [3]University of Florida, Gainesville, FL*

WP 435   **Five Easy Metrics of Data Quality for LC-MS Based Global Metabolomics**; Daniel Raftery[1]; Xinyu Zhang[2]; Jiyang Dong[3]; *[1]UW Medicine, SLU, Seattle, WA; [2]University of Washington, Seattle, WA; [3]Xiamen University, Xiamen, China*

WP 436   **Untargeted Metabolomics of Soil Extracts Using Parallel HILIC-RPLC LC-MS/MS with Stacked Injections: Study of Cheatgrass-Crested Wheatgrass Interaction**; Mitch Helling[1]; Gordon Custer[2]; Linda Van Diepen[2]; Franco Basile[1]; *[1]Department of Chemistry, University of Wyoming, Laramie, Wyoming; [2]Department of Ecosystem Science and Management, University of Wyoming, Laramie, Wyoming*

WP 437   **Metabolomic profiling of colorectal cancer using a dual-channel microphysiological model system**; Sujatha Chilakala[1]; Carly Strelez[1]; Ah Young Yoon[1]; Shannon Mumenthaler[1]; Jonathan E Katz[1]; *[1]Lawrence J. Ellison Inst for Transformative Medicine of University of Southern California, Los Angeles, California*

WP 438   **Investigating Iron Metabolism and Redox Homeostasis in the Central Nervous System Following Subarachnoid Hemorrhage**; Gardenia Pacheco[1]; Daniel Morris[2]; Christopher Ziegler[2]; Joao Gomes[3]; Leah P Shriver[2]; *[1]University of Akron, Akron, OH 44325; [2]University of Akron, Akron, OH; [3]Cleveland Clinic, Cleveland, OH 44195*

WP 439   **Metabolomics approach reveals dysbiosis in the gut microbiota by Salmonella infection**; Yongseok Kim[1]; Maryam Baniasad[1]; Anice Sabag-Daigle[1]; Michael T. Shaffer[2]; Kelly C. Wrighton[2]; Brian M.M. Ahmer[1]; Vicki H Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Colorado State University, Fort Collins, CO*

WP 440   **High Resolution Mass Spectrometry Characterization of Essential Oil and Extractives from Norway Spruce buds**; Omolara Mofikoya[1]; Marko Mäkinen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, Joensuu, Finland*

WP 441   **Getting the most out of GC-HRMS data using novel R-based software tools**; Carsten Jaeger[1]; Jan Lisec[1]; *[1]Federal Institute for Material Research and Testing, Berlin, Germany*

WP 442   **Metabolomics study of klk8 deficient mouse with different instruments and ionization/detection methods**; Lukáš Kučera[1]; Ashkan Zareie[1]; Kryštof Klíma[1]; Vendula Novosadová[1]; Matthias Witt[2]; Heino Heyman[3]; Radislav Sedláček[1]; *[1]Czech Centre for Phenogenomics, Prague, Czech Republic; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

WP 443   **Discovering variation of secondary metabolite diversity and relationship with antioxidant activities in Salicornia using Trapped Ion-Mobility Time-of-Flight (timsTOF) Mass Spectrometry**; Marcus Ehlert[1]; Christopher Aboo[1]; Verena Tellstroem[2]; Mette Hedegaard Thomsen[1]; Allan Stensballe[1]; *[1]Aalborg University, Aalborg, Denmark; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 444   **Untargeted UHLC-HR-QTOF-MS metabolomics study to unravel metabolites controlling wood formation in aspen trees**; Magdalene A. Reinkensmeier[1]; Ilara G.F. Budzinski[2]; Thomas Moritz[3, 4]; *[1]Bruker Daltonics, Bremen, Germany; [2]Umeå Plant Science Centre, Department of Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; [3]Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; [4]Novo Nordisk Foundation Centre for Basic Metabolic Research, University of Copenhagen, Copenhagen, Denmark*

WP 445   **LC-MS-Based analysis revealed different metabolic profiles in spent culture media of human embryos with distinct morphology, karyotype and implantation outcomes**; Alina Gamisonia[1, 2]; Chupalav Eldarov[1, 3]; Vitaliy Chagovets[1]; Luiza Ibragimova[1]; Veronika Smol`nikova[1]; Elena Kalinina[1]; Victor Zgoda[4]; Mikhail Bobrov[1, 2]; *[1]National Medical Research Center for Obstetrics, Gynecology and Perinatology, Moscow, Russia; [2]Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, RAS,, Moscow, Russia; [3]Belozersky Institute Of Physico-Chemical Biology, Moscow, Russia; [4]Institute of Biomedical Chemistry RAMS, Moscow, Russia*

WP 446   **Mapping the Chemical Diversity of a Freshwater Cyanobacterial Library for Enhanced Drug Discovery using Informatic Tools**; Lydia Davis[1]; Peter Sullivan[1]; Steven Kurina[1]; Joanna E. Burdette[1]; Jimmy Orjala[1]; *[1]College of Pharmacy at the University of Illinois at Chicago, Chicago, IL*

WP 447   **Metabolic profiling of Saccharomyces cerevisiae in response to deletions of genes involved in the glucose repression pathway**; April Miguez[1]; Mark Styczynski[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

WP 448   **2D Standard Addition Method for Estimation of the Number of Metabolites from the Features Detected using Untargeted RPIP LC-HRMS method**; Ruichuan Zhang[1]; Thomas Rydzak[2]; Ryan A Groves[2]; *[1]Independent Researcher, Calgary, AB; [2]University of Calgary, Calgary, AB*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES II
WP 449-462

WP 449   **Expanding the detection and discovery of ribonucleoside modifications by higher-energy collisional dissociation mass spectrometry (HCD-MS)**; Manasses Jora[1]; Peter A. Lobue[1]; Robert L. Ross[1]; Ningxi Yu[1];

Daniel Corcoran[1]; Ruoxia Zhao[1]; Scott Abernathy[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH*

WP 450 **Use of Ion-Mobility Mass Spectrometry to Determine Fluoroalcohol-induced Alterations in the Secondary Structure of Oligonucleotides**; J. Michael Sutton[1]; Michael G Bartlett[1]; [1]*University of Georgia, Athens, GA*

WP 451 **Ultrasensitive determination of rare modified nucleotides based on novel hydrazine labelling reagents**; Yue Yu[1]; Fang Yuan[1]; Xin Zheng[2]; Xin-ge Cui[2]; Yingling Zhou[1]; Xin-Xiang Zhang[3]; [1]*Peking University, College of Chemistry, Beijing, China; [2]Union Medical College Hospital, Beijing, China; [3]Peking University, Haidian, China*

WP 452 **Oligonucleotide Analysis via Microchip CE-MS**; Ashley Bell[1]; Erin A Redman[1]; J. Scott Mellors[1]; [1]*908 Devices, Inc., Carrboro, NC*

WP 453 **Differentiation of Oligonucleotide Diastereoisomeric Distributions by NH4+/K+ Complexation RP-HPLC MS**; Stilianos G. Roussis[1]; Isaiah Cedillo[1]; Claus Rentel[2]; [1]*Ionis Pharmaceuticals, Inc., Carlsbad, CA; [2]Ionis Pharmaceuticals, Inc, Carlsbad, CA*

WP 454 **Stable isotope labeling with nucleosides in cell culture as an approach to RNA modification dynamics**; Mayu Tezuka[1]; Yuko Nobe[1]; Yuka Yamaki[1]; Yoshio Yamauchi[1]; Hiroshi Nakayama[2]; Masato Taoka[1]; [1]*Tokyo Metropolitan University., Hachioji, Japan; [2]RIKEN Center for Sustainable Resource Science, Wako, Japan*

WP 455 **Evaluation of TOF MS Approaches for the Quantitation of Qligonucleotides**; Esme Candish[1]; Dilip Reddy[2]; Ji Jiang[3]; Sean Mc Carthy[2]; [1]*SCIEX, Framingham, MA; [2]Sciex, Framingham, MA; [3]SCIEX, Redwood Shores, California 1201*

WP 456 **Negative-Ion Mode Data Independent Acquisition for an RNA Centric Approach to Analysis of UV Photo-Crosslinked Ribonucleoproteins by Mass Spectrometry**; Carson W Szot[1]; Tracy Hodges[2]; Laura Snyder[2]; Sarah C. Keane[1]; Kristina Hakansson[2]; [1]*University of Michigan, Ann Arbor, MI; [2]University of Michiagan, Ann Arbor, MI*

WP 458 **Characterization of phosphate- and phosphorothioate-linked nucleic acids by 213-nm ultraviolet photodissociation tandem mass spectrometry**; Hiroshi Nakayama[1]; Daisuke Higo[2]; Masami Koike[1]; Masato Taoka[3]; [1]*RIKEN CSRS, Wako, Japan; [2]Thermo Fisher Scientific, Yokohama, Japan; [3]Tokyo Metropolitan University., Hachioji, Japan*

WP 459 **Qualitative and Quantitative analysis of Phosphorothioate Oligonucleotides Using a Quadrupole-Time-of-Flight Mass Spectrometer**; Noriko Kato[1]; Tairo Ogura[1]; Yusuke Inohana[1]; Masaki Yamada[1]; Toshiya Matsubara[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

WP 460 **Recent advances in mass spectrometry of oligonucleotides**; Michael G. Bartlett[1]; J. Michael Sutton[1]; Vidya Annavarapu[1]; Guilherme Jendiroba Guimaraes[1]; [1]*University of Georgia, Athens, GA*

WP 461 **Diol-based HILIC Chromatography and HRAM Mass Spectrometry for the Analysis of Double-stranded Oligodeoxynucleotides Crosslinked by the Bacterial Genotoxin Colibactin**; Alessia Stornetta[1]; Peter W. Villalta[1]; Erik S. Carlson[2]; Emily P. Balskus[2]; Silvia Balbo[1, 3]; [1]*University of Minnesota Masonic Cancer Center, Minneapolis, MN; [2]Department of Chemistry and Chemical Biology, Harvard University, Boston, MA; [3]Division of Environmental Health Sciences, University of Minnesota, Minneapolis, MN*

WP 462 **Mass Spectrometric Approaches for the Structural Characterization of Chemically Targeted PreQ1 Riboswitches**; Christopher C. Lai[1]; Desta D. Bume[1]; John S. Schneekloth, Jr.[1]; James A. Kelley[1]; [1]*National Institutes of Health, Frederick, MD*

PHOSPHOPEPTIDES: QUANTITATIVE ANALYSIS
WP 463-471

WP 463 **Tandem Mass Tag Approach Utilizing Pervanadate BOOST Channels Delivers Deeper Quantitative Characterization of the Tyrosine Phosphoproteome**; Xien Yu Chua[1]; Theresa Mensah[1]; Timothy Aballo[1]; Samuel G Mackintosh[2]; Ricky Edmondson[2]; Arthur Salomon[1]; [1]*Brown University, Providence, RI; [2]University of Arkansas for Medical Sciences, Little Rock, AR*

WP 464 **Phosphorylation ratio determination in fresh frozen and formalin-fixed paraffin embedded tissue with targeted mass spectrometry**; Lona Zeneyedpour[1]; Christoph Stingl[1]; Lennard J.M. Dekker[1]; Dana A.M. Mustafa[1]; Johan M. Kros[1]; Theo M. Luider[1]; [1]*Erasmus Medical Center, Rotterdam, Netherlands*

WP 465 **Label-free Quantification Analysis of C-terminal Domain Phosphorylation using 193 nm Ultraviolet Photodissociation Mass Spectrometry**; Edwin Escobar[1]; Mukesh Kumar[1]; Yan Zhang[1]; Jennifer Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 466 **Facile determination of phosphorylation sites in peptides using two-dimensional mass spectrometry and UVPD**; Johanna Paris[1]; Tomos E Morgan[1]; Alina Theisen[1]; Bryan P. Marzullo[1]; Anisha Haris[1]; Christopher A. Wootton[1]; Mark P. Barrow[1]; John O'hara[2]; Peter B O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom; [2]UCB, Slough, United Kingdom*

WP 468   **Deep Profiling of Tyrosine Phosphorylation in Gastric Cancer Cells**; <u>Matthew Willetts</u>[1]; Shourjo Ghose[2]; Charles L Farnsworth[3]; Alissa J. Nelson[3]; Yiying Zhu[3]; Kimberly L Lee[3]; *[1]Bruker, Billerica, MA; [2]Bruker Daltonics, Billerica, MA; [3]Cell Signaling Technology, Danvers, MA*

WP 469   **Targeted proteomic characterization of the AKT/mTOR pathway through analysis of clinically derived samples**; <u>Rowan Matney</u>[1]; Kratika Singhal[1]; Fang Liu[1]; Sarah Trusiak[2]; Emily Chen[2]; Ryan D. Leib[1]; Allis S. Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA; [2]Thermo Fisher Precision Medicine Science Center, Cambridge, MA*

WP 470   **Personalized phosphoproteomics of insulin action potentiated by exercise**; <u>Elise Needham</u>[1]; Janne Hingst[2]; Benjamin Parker[3]; Guang Yang[4]; Jonathan Oakhill[5]; Christian Pehmøller[6]; Jørgen F.p. Wojtaszewski[7]; Sean Humphrey[4]; David E. James[4]; *[1]Charles Perkins Centre, School of Life and Environmental Sciences, The University of Sydney, Sydney, Australia; [2]Section of Molecular Physiology, Department of Nutrition, Exercise and Sports, University of Copenhagen, Copenhagen, Denmark; [3]Department of Physiology, School of Biomedical Sciences, University of Melbourne, Parkville, Australia; [4]Charles Perkins Centre, School of Life and Environmental Sciences, University of Sydney, Sydney, Australia; [5]Metabolic Signalling Laboratory, St Vincent's Institute of Medical Research, School of Medicine, University of Melbourne, Parkville, Australia; [6]Internal Medicine Research Unit, Pfizer Global Research and Development, Cambridge, MA, Brunei, Cambridge, MA; [7]Section of Molecular Physiology, Department of Nutrition, Exercise and Sports, University of Copenhagen,, Copenhagen, Denmark*

WP 471   **Phospho-proteomic Characterization of IL-2 and IL-15 Signaling in NK-92 cells**; <u>Melanie A. Macmullan</u>[1]; Pin Wang[1]; Nicholas A. Graham[1]; *[1]University of Southern California, Los Angeles, CA*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS
WP 472-493

WP 472   **N-Glycan Profiling Using RapiFluor-MS N-Glycan Kit in Biopharmaceutical Discovery and Development**; <u>Yanyan Lu</u>[1]; Ying Zhou[1]; *[1]Alkermes, Inc, Waltham, MA*

WP 473   **A holistic approach to comprehending the in vivo intact stability of novel modalities using LC-MS and capillary electrophoresis-based methods**; <u>Hannah Chi</u>[1]; Cong Wu[1]; Phillip Chu[1]; Hilda Hernandez-Barry[1]; William Sawyer[1]; Neha Srikumar[2]; Brian Roper[1]; Thomas Niedringhaus[1]; Adrian Papas[3]; John Tran[1]; *[1]Genentech, South San Francisco, CA; [2]University of Pennsylvania, Philadelphia, PA; [3]ProteinSimple, San Jose, California*

WP 474   **Automated Workflow for Proteoforms Characterization and Quantification of Intact Monoclonal Antibodies by CEX-MS**; <u>Angela Criscuolo</u>[1]; Marc Guender[2]; Sara Carillo[3]; Florian Füssl[3]; Ken Cook[4]; Jonathan Bones[3]; *[1]Thermo Fisher Scientific, Dreieich, Germany; [2]Thermo Fisher Scientific, reinach, Switzerland; [3]National Institute of Bioprocessing Research and Training, Dublin, Ireland; [4]Thermo Fisher Scientific, Hemel, United Kingdom*

WP 475   **Enhanced Detection of Host Cell Proteins enabled by use of Collisional Cross Sections**; <u>Stuart Pengelley</u>[1]; Christine Paul[2]; Eckhard Belau[1]; Waltraud Evers[1]; Tim Welsink[2]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]InVivo BioTech Services, Hennigsdorf, Germany*

WP 476   **Dietary Biotin Interference in Hybrid LBA-LC-MS/MS Assays: Characterization, Impact, and Recommendations**; <u>Jean-Nicholas Mess</u>[1]; Kevork Mekhssian[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC*

WP 477   **Meeting the Challenges of Implementing the Multi-Attribute Method (MAM) in Regulated/Non-Regulated Environments**; <u>Nilini Ranbaduge</u>[1]; Ying Qing Yu[2]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corps, Milford, MA*

WP 478   **Parallel Reaction Monitoring (PRM) Quantification of Herceptin and Trastuzumab N-Glycans**; <u>Joshua Shipman</u>[1]; Jason Rodriguez[1]; Connie Ruzicka[2]; David Keire[1, 2]; Kang Chen[1]; Hongbin Zhu[1]; *[1]Division of Complex Drug Analysis, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO; [2]Division of Pharmaceutical Analysis, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO*

WP 479   **Automated, workflow-based quality monitoring of biotherapeutics: Implementing MS-based Multi-attribute Method (MAM) approaches**; <u>Maurizio Bronzetti</u>[1]; Jonathan Jones[2]; Peter Haberl[3]; Catherine Evans[4]; *[1]Genedata Inc, San Francisco, CA; [2]Genedata Ltd, Cambridge, United Kingdom; [3]Genedata GmbH, Munich, Germany; [4]Genedata AG, Basel, Switzerland*

WP 480   **Integrated characterization and screening workflows to simplify the design of MAM methods**; Guillaume Tremintin[1]; Detlev Suckau[2]; Yue Ju[1]; <u>Anjali Alving</u>[3]; *[1]Bruker Daltonics, San Jose, CA; [2]Bruker Daltonic GmbH, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

WP 481   **Highly sensitive LC-MS/MS workflow for targeted quantification of host cell proteins**; Lei Xiong[1]; <u>Yi Zhang</u>[1]; Ian Moore[2]; *[1]SCIEX, Redwood Shores, CA; [2]SCIEX, Concord, ON*

WP 482   **A Fast and Simple Immuno-mass Spectrometry Based Method Enables Universal Preclinical Bioanalysis for IgG-1 Type mAb**; <u>Jiashu Tang</u>[1]; Yue Zhou[1]; *[1]Thermo Fisher Scientific, Shanghai, China, shanghai, China*

WP 484   **Understanding the Proteomic Differences Between Primary and Super-charged Natural Killer Cells**; Lucy Wanrong Gao[1]; Meng-Wei Ko[2]; Anahid Jewett[2, 3]; Julian Whitelegge[1]; *[1]The Pasarow Mass Spectrometry Laboratory, The Jane and Terry Semel Institute for Neuroscience and Human Behavior, David Geffen School of Medicine, UCLA, Los Angeles, CA; [2]Division of Oral Biology and Oral Medicine, The Jane and Jerry Weintraub Center for Reconstructive Biotechnology, UCLA,, Los Angeles, CA; [3]The Jonsson Comprehensive Cancer Center, UCLA School of Dentistry and Medicine,, Los Angeles, CA*

WP 485   **Proteomic Characterization of Amyloid-Laden Brain Regions: A Condition with Compromised Proteostasis**; Arun Upadhyay[1]; Jeffrey Savas[1]; *[1]Northwestern University, Chicago, IL*

WP 486   **A universal LCMS workflow for therapeutic monoclonal antibody bioanalysis**; Li Sun[1]; Lisa O'callaghan[1]; Daniel Spellman[1]; *[1]PPDM Bioanalytics, Merck & Co., Inc., West Point, PA*

WP 487   **LC-MS/MS method development of aflibercept using Fab-selective proteolysis nSMOL technology**; Nozomi Maeshima[1]; Kenichi Aizawa[2]; Manami Kobayashi[1]; Kota Ishioka[1]; Takashi Shimada[3]; Junichi Masuda[1]; *[1]Shimadzu Corporation, Hadano, Japan; [2]Jichi Medical University, Shimotsuke, Japan; [3]Shimadzu Scientific Instruments, Bothell, WA*

WP 488   **Bioanalytical Strategies for Comprehensive Pharmacokinetic and Catabolism Assessments of ADCs, A Case Study with MEDI3726**; Eric Ma[1]; Michael P Waldron[1]; Marlking Peay[1]; Moucun Yuan[1]; Omnia Ismaiel[1]; William R. Mylott[1]; Yue Huang[2]; Christopher Del Nagro[2]; Kemal Balic[2]; Meina Liang[2]; Lorin Roskos[2]; Anton I Rosenbaum[2]; *[1]PPD Laboratories, Richmond, VA; [2]Clinical Pharmacology & Quantitative Pharmacology, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, South San Francisco, California*

WP 489   **A highly efficient LC-MS based techniques for targeted quantification of biotherapeutics and protein marker levels in FFPE tumors**; Chao Xue[1]; Jie Pu[1]; Yang Liu[1]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

WP 490   **LC-MS Based Quantification of Therapeutic Monoclonal Antibody in Human Serum and Evaluation of Assay Sensitivity, Selectivity and Specificity**; Yao Shi[1]; Brendan Powers[1]; David Good[1]; Shashank Gorityala[1]; Zachariah Herendeen[1]; Yongle Pang[1]; Aaron Ledvina[1]; Stephanie Cape[1]; *[1]Covance, Madison, WI*

WP 491   **Comprehensive Investigation on Antibody-Drug Conjugates Induced Ocular Toxicity Using Novel LC-MS-based Strategies**; Xiaoyu Zhu[1]; Min Ma[1, 2]; Ming Zhang[1]; Bo An[1]; Shihan Huo[1]; Yang Qu[1]; Jie Pu[1]; Jun Qu[1, 3]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Institute, Buffalo, NY; [3]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

WP 492   **Accurate and Reliable Analysis of Antibody Biotherapeutics in Tissues using Novel Sample Treatment and LC/MS Strategies**; Xinxin Yang[1, 2]; Chao Xue[1, 2]; Ming Zhang[1, 2]; Yang Qu[1, 2]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]Center of Excellence in Bioinformatics and Life Sciences, Buffalo, New York*

WP 493   **Narrow-window-Q1 Isolation LC-SRM/MS Enables Isotope-specific Transitions with Improved Selectivity/sensitivity for Protein Biomarkers Quantification**; Shihan Huo[1]; Jie Pu[1]; Qingqing Shen[1]; Ming Zhang[1, 2]; Xiaoyu Zhu[1]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

PROTEINS: PTMS II
WP 494-510

WP 494   **CobB serves as a lysine de-2-hyroxyisobutyrylation enzyme to regulate glycolysis and cell growth in bacteria**; Kai Zhang; *Tianjin Medical University, Tianjin, China*

WP 495   **Comparing 22 popular phosphoproteomics pipelines for peptide identification and site localization**; Marie Locard-Paulet[1]; David Bouyssié[2]; Carine Froment[2]; Odile Burlet-Schiltz[2]; Lars J Jensen[1]; *[1]Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; [2]Institut de Pharmacologie et de Biologie Structurale, Université de Toulouse, CNRS, Toulouse, France*

WP 496   **A method for occupancy quantification of site-specific lysine post-translational modifications**; Martin Mathay[1]; Juan D. Chavez[1]; Jimmy K Eng[1]; James E Bruce[1]; *[1]University of Washington, Seattle, WA*

WP 497   **A quantitative proteomics approach to investigate processes related to mitophagy in human cells**; Katharina Zittlau[1]; Anna Lechado-Terradas[2]; Sven Geisler[3]; Nicolas Nalpas[1]; Philipp Kahle[3]; Boris Macek[1]; *[1]Quantitative Proteomics and Proteome Center Tuebingen, Interfaculty Institute for Cell Biology, University of Tuebingen, Auf der Morgenstelle 15, Tuebingen, Germany; [2]Functional Neurogenetics Department of Neurodegeneration, Hertie Institute for Clinical Brain Research and German Center for Neurodegenerative Diseases, Faculty of Medicine, University of Tuebingen Otfried-Müller-Strasse 27, Tuebingen, Germany; [3]Functional Neurogenetics Department of Neurodegeneration, Hertie Institute for Clinical Brain Research and German Center for Neurodegenerative Diseases, Faculty of Medicine, University of Tübingen Otfried-Müller-Strasse 27, Tuebingen, Germany*

WP 498   **Rapid assessment of protein structural heterogeneity using native LC/MS**; Wenhua Yang[1]; Igor A Kaltashov[1]; *[1]Univ. of Massachusetts/Chemistry Dept., Amherst, MA*

WP 499   **Identifying novel upstream kinases of the microtubule-associated protein Tau using fluorescence complementation mass spectrometry (FCMS)**; <u>Der-Shyang Kao</u>[1]; Yanyan Du[1]; W. Andy Tao[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West Lafayette*

WP 500   **Mining the Proteome for Sulfenic Acid Modifications with Cell permeable clickable trans-cyclooctenol (TCOl) chemical probes**; <u>Uthpala I Seneviratne</u>; *Pfizer Inc., Cambridge, MA*

WP 501   **Quantitative Top Down Proteomics Reveals Acetyltransferase Inhibition has differential effects on Histone Acetylation Dependent on Cellular Physiological State**; Lang Ding[1]; <u>Bethany C. Taylor</u>[1]; Amanda L. Wong[1]; Matthew V. Holt[1]; Tao Wang[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX*

WP 502   **Understanding the effect of nutrients on the epigenome**; <u>Arabella L Garcia</u>[1]; Peder J Lund[2]; Benjamin A Garcia[2]; *[1]Strath Haven High School, Wallingford, PA; [2]University of Pennsylvania School of Medicine, Philadelphia, PA*

WP 504   **Trapped Ion Mobility Spectrometry and PASEF Enables In-depth Characterization of Protein Ubiquitination from Human Cells**; Xiaoxian Du[1]; Jun Zhu[2]; Chen Bu[2]; Xianming Liu[1]; Ning Chen[3]; <u>Conor Mullens</u>[4]; Heiner Koch[5]; *[1]Bruker Daltonics, shanghai, China; [2]PTM Biolabs Inc., Hangzhou, China; [3]Bruker Daltonics, Beijing, China; [4]Bruker Daltonics, Billerica, MA; [5]Bruker Daltonic GmbH, Bremen, Germany*

WP 505   **PhoSSPair: An online deep learning-based tool to mine literature information on phosphorylation sites**; <u>Sara R. Savage</u>[1]; Yaoyun Zhang[2]; Eric J Jaehnig[1]; Hua Xu[2]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Melax Technologies, Houston, TX*

WP 506   **Reconstructing Protein Charge Heterogeneity from a Bottom-Up Approach**; Andrew Mahan[1]; Bo Zhai[1]; Robert Hepler[1]; Andrew Nichols[2]; Yong Joo Kil[2]; Eric Carlson[2]; <u>Hirsh Nanda</u>[1]; *[1]Janssen R&D LLC., Spring House, PA; [2]Protein Metrics, Cupertino, CA*

WP 507   **Highly Sensitivity Lysine Acetylation Profiling with Trapped Ion Mobility Spectrometry and PASEF**; Xianming Liu[1]; Jun Zhu[2]; Chen Bu[2]; Ning Chen[3]; Xiaoxian Du[1]; <u>Shourjo Ghose</u>[4]; Heiner Koch[5]; *[1]Bruker Daltonics, shanghai, China; [2]PTM Biolabs Inc., Hangzhou, China; [3]Bruker Daltonics, Beijing, China; [4]Bruker Scientific LLC, Billerica, MA; [5]Bruker Daltonics, Bremen, Germany*

WP 508   **Investigation of PTM changes in blood plasma proteome associated with AD and MCI**; <u>Maria Indeykina</u>[1, 2]; Natalia Zakharova[1, 2]; Anna Bugrova[1]; Alexander Brzhozovskiy[3]; Yana B. Fedorova[2, 4]; Svetlana I. Gavrilova[2, 4]; Alexey Kononikhin[2, 3]; Eugene (evgeny) Nikolaev[3]; *[1]Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow,, Russia; [2]Moscow Institute of Physics and Technology, Dolgoprudny, Russia; [3]Skolkovo Institute of Science and Technology, Moscow, Russia; [4]Mental Health Research Center, Russian Academy of Science, Moscow, Russia*

WP 509   **Sheathless Capillary Electrophoresis Coupled to Mass Spectrometry for Biopharmaceutical Characterization**; <u>Ruinan Yang</u>[1]; Gordon Nicol[1]; Chenhua Zhang[1]; Qiling Tang[1]; Jie Ding[1]; *[1]PPD, Middleton, WI*

WP 510   **Label-free quantification for top-down two-dimensional mass spectrometry**; Matthias Halper[1]; Marc-André Delsuc[2, 3]; Kathrin Breuker[1]; <u>Maria Van Agthoven</u>[1]; *[1]University of Innsbruck, Institute of Organic Chemistry, Innsbruck, Austria; [2]Institut de Génétique et de Biologie Moléculaire et Cellulaire, Illkirch-Graffenstaden, France; [3]CASC4DE, Strasbourg, France*

PROTEOMICS: INFECTIOUS DISEASES
WP 511-522

WP 511   **Proteomic and Phosphoproteomic Profiling of Praziquantel Treatment on Schistosoma mekongifor Investigation of Potential Parasiticidal Mechanisms.**; <u>Peerut Chienwichai</u>[1]; Poom Adisakwattana[2]; Tipparat Thiangtrongjit[3]; Yanin Limpanont[4]; Sumate Ampawong[5]; Onrapak Reamtong[3]; *[1]Faculty of Medicine and Public Health, HRH Princess Chulabhorn College of Medical Science, Chulabhorn Royal Academy, Bangkok, Thailand; [2]Department of Helminthology, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; [3]Department of Molecular Tropical Medicine and Genetics, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; [4]Department of Social and Environmental Medicine, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; [5]Department of Tropical Pathology, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand*

WP 512   **Expression and Purification as well as Mass Spectrometric and Immunoanalytical Characterization of the MBP-pfMSP119 Fusion Protein – Towards Malaria Screening**; <u>Kwabena F.M. Opuni</u>[1, 2]; Cornelia Koy[1]; Bright Danquah[1]; Maren Reepmeyer[1]; Manuela Ruß[1]; Peter Lorenz[3]; Hans-Jürgen Thiesen[3]; Moritz Weresow[4]; Astrid Alef[4]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, University Medicine Rostock and University of Rostock, Schillingallee 69, Rostock, Germany; [2]Department of Pharmaceutical Chemistry, School of Pharmacy, College of Health Science, University of Ghana, Accra, Ghana; [3]Institute for Immunology, University Medicine Rostock, Schillingallee 70, Rostock, Germany; [4]I&L Biosystems GmbH, Königswinterer Str. 409, Königswinterer, Germany*

WP 513   **Saving millions of lives with 50.000 quantified proteomes of bacterial pathogens**; <u>Annegret Ulke-Lemee</u>[1]; Jenna Poelzer[1]; Mario Valdez Tresanco[1]; Soren Wacker[1]; Thomas Rydzak[1]; Sergei Noskov[1]; Ian Andrew Lewis[1]; *[1]University of Calgary, Calgary, AB*

WP 514 **Proteogenomics towards the characterization of antimicrobial peptide resistance patterns in Escherichia coli**; Patric W. Sadecki[1]; Leslie M. Hicks[1]; [1]*UNC - Chapel Hill, Chapel Hill, NC*

WP 515 **Bottom-up Proteomics Reveals the Impact of Salmonella Infection on the Gut Environment**; Maryam Baniasad[1]; Yongseok Kim[1]; Anice Sabag-Daigle[1]; Michael T. Shaffer[2]; Kelly C. Wrighton[2]; Brian M.M. Ahmer[1]; Vicki H. Wysocki[1]; [1]*The Ohio State University, Columbus, OH;* [2]*Colorado State University, Fort Collins, CO*

WP 516 **Limited Tryptic Digestion-Isotope Dilution Mass Spectrometry (LTD-IDMS):A regent-free analytical assay to quantify hemagglutinin of H5N1 influenza vaccine material**; Hans C Cooper[1]; Yuhong Xie[2]; William Sutton[1]; Giuseppe Palladino[2]; John R Barr[1]; Ethan C. Settembre[2]; Yingxia Wen[2]; Tracie Williams[1]; [1]*Centers of Disease Control and Prevention (CDC), Atlanta, GA;* [2]*Seqirus, Cambridge, MA 02139*

WP 517 **Proteomic approaches for the epidemiology and diagnosis of tick-borne diseases**; Paola Cantero[1]; Pierre Boyer[2]; Josiane Saade[1]; Nathalie Boulanger[2]; Benoît Jaulhac[2]; Maria Kazimirova[3]; José De La Fuente[4, 5]; Marie Jalovecka[6, 7]; Laurence Ehret-Sabatier[1]; [1]*Laboratoire de Spectrométrie de Masse BioOrganique, UMR 7178, CNRS, Université de Strasbourg, Strasbourg, France;* [2]*UR7290, Virulence bactérienne précoce : groupe Borrelia, Fédération de Médecine Translationnelle de Strasbourg, Université de Strasbourg, Strasbourg, France;* [3]*Institute of Zoology, Slovak Academy of Sciences, Bratislava, Slovakia;* [4]*SaBio, IREC, Ronda de Toledo s/n, Ciudad Real, Spain;* [5]*Department of Veterinary Pathobiology, Center for Veterinary Health Sciences, Oklahoma State University, Stillwater, Oklahoma;* [6]*Institute of Parasitology, Biology Centre of the Czech Academy of Sciences, Ceske Budejovice, Czech Republic;* [7]*Faculty of Science, University of South Bohemia, Ceske Budejovice, Czech Republic*

WP 518 **New strategy for bacterial species identification in Urinary Tract Infection using Artificial Intelligence on Ultrafast LC-MSMS-DIA runs**; Florence Roux-Dalvai[1]; Mickaël Leclercq[1]; Marion Narbeburu[1]; Tabiwang N. Arrey[2]; Nicolai Bache[3]; Clarisse Gotti[1]; Claire Dauly[2]; Dorte B. Bekker-Jensen[3]; David Bouyssié[4]; Maurice Boissinot[5]; Michel G. Bergeron[5]; Arnaud Droit[1]; [1]*Proteomics platform and Computational Biology Laboratory - CHU Québec Université Laval Research Center, Québec, QC;* [2]*Thermo Fisher Scientific, Bremen, Germany;* [3]*Evosep Biosystems, Odense, Denmark;* [4]*Institut de Pharmacologie et de Biologie Structurale, Université de Toulouse, CNRS, Toulouse, France;* [5]*Infectiology Research Center - CHU Québec Université Laval Research Center, Québec, QC*

WP 519 **Utilizing Cross-Linking Mass Spectrometry to Rapidly Dissect Host:Pathogen Interactions of High-Containment Diseases**; Nathen Bopp[1]; William Russell[1]; [1]*University of Texas Medical Branch at Galveston, Galveston, TX*

WP 520 **Quantitative Proteomics Reveals a Multifactorial Mechanism of Antifungal Drug Resistance**; Margarita Semis[1]; Daniel Roeth[1]; Elizabeth Abby Henderson[1]; Markus Kalkum[1]; [1]*City of Hope, Duarte, CA*

WP 521 **HIV Phosphorylation Site Investigation Using MALDI-LTQ**; Andre D. Dunkley[1]; Kevin J. Mark[1, 2]; Pratikkumar Rathod[1, 2]; Emmanuel Chang[2, 3]; [1]*Department of Natural Sciences, LaGuardia Community College;, Long Island City, NY;* [2]*Department of Chemistry, York College, Jamaica, NY;* [3]*Graduate Center/City University of New York, New York, NY*

WP 522 **A Proteomic Investigation of Antibiotic Resistance and Susceptibility in Mycobacterium abscessus**; Sung Hwan Yoon[1]; Meena Rajagopal[2]; Adrian Zelazny[2]; Aleksandra Nita-Lazar[1]; [1]*NIH/NIAID, Bethesda, MD;* [2]*NIH/CC/DLM, Bethesda, MD*

PROTEOMICS: QUANTITATIVE II
WP 523-536

WP 523 **TMT-Integrator: An efficient analysis and multi-level report generation for labeling-based proteomics experiments**; Hui-Yin Chang[1]; Felipe Da Veiga Leprevost[2]; Weiping Ma[3]; Pei Wang[3]; Bo Wen[4]; Bing Zhang[4]; Alexey I. Nesvizhskii[2]; [1]*University of Michigan, Ann Arbor, MI;* [2]*University of Michiagan, Ann Arbor, MI;* [3]*Icahn School of Medicine at Mount Sinai, New York, NY;* [4]*Baylor College of Medicine, Houston, TX*

WP 524 **Temporal Mitochondrial Proteomic Analysis of Pancreatic β-Cells in Response to Lipotoxicity and Glucolipotoxicity**; Min Li[1]; Junjie Hou[1]; [1]*Institute of Biophysics, CAS, Beijing, China*

WP 525 **Targeted Profiling of Epitranscriptomic Reader, Writer and Eraser Proteins in Radioresistant Breast Cancer Cells**; Tianyu Qi[1]; Weili Miao[1]; Yinsheng Wang[1]; [1]*UC RIVERSIDE, Riverside, CA*

WP 526 **Label free pharmacoproteomic assays enabled the discovery of cellular pathways involved in the survival of MCF7 and K567 cancer cells**; Cristina C Clement[1]; Shu-Yuan Cheng[2]; Monika Dzieciatkowska[3]; Elise Champeil[2]; [1]*Weill Cornell Medicine, New York, NY;* [2]*Department of Sciences, John Jay College of Criminal Justice, City University of New York, New York, NY;* [3]*Biological Mass Spectrometry Core Facility, University of Colorado Denver, Aurora, Denver, Colorado*

WP 527 **Quantitative Proteomics Analysis of the Aminoglycoside Producer Streptomyces tenebrarius**; Darwin Linardi[1]; Tingyu Pan[2]; Yi Yu[2]; Henry Lam[3]; [1]*The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong;* [2]*Wuhan University, Wuhan, China;* [3]*The Hong Kong University of Science and Technology (HKUST), Clear Water Bay, Hong Kong*

WP 528   **Investigation and Characterization of the Jumping Translocation Breakpoint (JTB) Protein using Mass Spectrometry based Proteomics**; Madhuri Jayathirtha[1]; Devika Channaveerappa[1]; Kangning Li[1]; Costel Darie[1]; [1]*Clarkson University, Potsdam, NY*

WP 529   **Reducing compression effects and expanding the multiplex capabilities on a timsTOF Pro with PASEF**; Michael Krawitzky[1]; Christopher Adams[1]; Matt Willetts[2]; Tharan Srikumar[2]; [1]*Bruker Daltonics, San Jose, CA;* [2]*Bruker Daltonics, Billerica, MA*

WP 530   **Proteomic Analysis of Large Cohorts with a Micro Pillar Array Capillary Column**; Simion Kreimer[1]; Qin Fu[1]; Angela Mc Ardle[1]; Kimia Sobhani[1]; Cory Bystrom[1]; Jennifer Van Eyk[1]; [1]*Cedars-Sinai Medical Center, Los Angeles, CA*

WP 531   **Quantitative Proteomics of Cytosolic Proteins Derived from Temozolomide-resistant Glioma**; Milan Teraiya[1]; Helene Perreault[1]; Vincent Chen[2]; [1]*University of Manitoba, Department of Chemistry, Winnipeg, Manitoba;* [2]*Brandon University, Department of Chemistry, Brandon, Manitoba*

WP 532   **Quantitative Proteomic and Phosphoproteomic Analysis of 36 Breast and Ovarian Cancer Cell Lines**; Gary A. Bradshaw[1]; Robyn Eisert[1]; Caitlin E. Mills[1]; Maulik Nariya[1]; Marian Kalocsay[1]; Peter K. Sorger[1]; [1]*Harvard Medical School, Boston, MA*

WP 533   **Comparative evaluation of different plasma preparation techniques by TIMS TOF Pro instrument for quantification of up to 1000 plasma proteins**; Alexander Brzhozovskiy[1]; Alexey Kononikhin[1, 2]; Anna Bugrova[3]; Maria Indeykina[2, 3]; Natalia Zakharova[2, 3]; Christoph H. Borchers[1, 4]; Eugene (evgeny) Nikolaev[1, 5]; [1]*Skolkovo Institute of Science and Technology, Moscow, Russia;* [2]*Moscow Institute of Physics and Technology, Dolgoprudny, Russia;* [3]*Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow,, Russia;* [4]*McGill University, Montreal, QC;* [5]*Institute of Energy Problems of Chemical Physics Russian Academy of Sc., Moscow, Russia*

WP 534   **New Quadrupole-Ion Trap-Orbitrap Mass Spectrometer Combined with Real Time Search Enhances Proteome Coverage and Quantification Accuracy in Multiplexing Workflows**; Xiangyun Yang[1]; Xiujie Sun[1]; Yue Zhou[1]; [1]*Thermo Fisher Scientific, Shanghai, China*

WP 535   **Establishing a Proteomics Pipeline for the Developing Proto-Vertebrate Ciona intestinalis**; Alexander Frese[1]; Andrea Mariossi[1]; Michael Levine[1]; Martin Wuhr[1]; [1]*Princeton University, Princeton, NJ*

WP 536   **Comparison of Protein Quantification in human plasma by TMT and DIA workflows**; Renny Shang-Lun Lan[1, 2]; Aaron J. Storey[2]; Austin L. Brown[3]; Stefan H. Graw[2]; Samuel G. Mackintosh[2]; Stephanie D. Byrum[2]; Ricky D. Edmondson[2]; [1]*Arkansas Children's Nutrition Center, Little Rock, AR;* [2]*University of Arkansas for Medical Sciences, Little Rock, AR;* [3]*Baylor College of Medicine, Houston, Texas*

PROTEOMICS: TOP DOWN ANALYSIS I
WP 538-547

WP 538   **Laser Ablation Microsampling for Top-Down Mass Spectrometry**; Remilekun O. Lawal[1]; Fabrizio Donnarumma[1]; Kermit Murray[1]; [1]*Louisiana State University, Baton Rouge, LA*

WP 539   **Towards an optimized sample preparation protocol for denaturing top-down proteomics of complex proteomes**; Zhichang Yang[1]; Xiaojing Shen[1]; Daoyang Chen[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

WP 540   **Integration of 193 nm ultraviolet photodissociation and fragment ion protection to improve the sequence coverage of large proteins**; Sean D Dunham[1]; James D. Sanders[1]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 541   **Profiling of Lipid-transfer Proteins from Plasma Using Miniaturized AF4 Coupled with ESI-MS**; Jin Yong Kim[1]; Myeong Hee Moon[1]; [1]*Yonsei University, Seoul, South Korea*

WP 542   **Comprehensive characterization of antibody drug conjugates by CESI-MS**; Andras Guttman[1, 2]; Bryan R Fonslow[3]; Gabor Jarvas[2]; [1]*Sciex, Brea, CA;* [2]*University of Debrecen, Debrecen, Hungary;* [3]*The Scripps Research Institute, La Jolla, CA*

WP 543   **Adaptation of Native GELFrEE for HDL Particle Size Subtype Separation and Differential Apolipoprotein Proteoform Quantification**; Cameron Lloyd-Jones[1]; Henrique dos Santos Seckler[2]; Allan Sniderman[3]; Philip D Compton[2]; John T. Wilkins[4]; Neil L Kelleher[2]; [1]*Northwestern University, Evanston, IL;* [2]*Northwestern University, Evanston, IL/60208;* [3]*McGill University, Montreal, QC;* [4]*Northwestern University, Chicago, IL*

WP 544   **Activated-Ion Electron Transfer Dissociation Enables Electron-Based Dissociation Following Proton Transfer Charge Reduction**; Josh Hinkle[1]; Christopher Mullen[1]; Jean M Lodge[2]; Romain Huguet[1]; Michael S Westphall[2]; Joshua J Coon[2]; John E.P. Syka[1]; [1]*ThermoFisher Scientific, San Jose, CA;* [2]*University of Wisconsin-Madison, Madison, Wisconsin*

WP 545   **MASH Explorer, A Universal and Comprehensive Software for Top-down Proteomics Empowered by Machine Learning Methods**; Sean J. Mcilwain[1]; Zhijie Wu[2]; Kent Wenger[3, 4]; Molly Wetzel[3, 4]; Jake A. Melby[5];

Xiaowen Liu[6, 7]; Ruixiang Sun[8]; Irene M. Ong[1, 9]; Ying Ge[3, 4, 5]; [1]*Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222;* [3]*Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI;* [4]*Human Proteomics Program, School of Medicine and Public Health, Madison, WI;* [5]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [6]*Department of BioHealth Informatics, Indianapolis, IN - Indiana;* [7]*Center for Computational Biology and Bioinformatics, Indiana University, Indianapolis, IN;* [8]*Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China;* [9]*Department of Obstetrics and Gynecology, University of Wisconsin, Madison, WI*

WP 546   **Facilitating User Defined Proteomics Search Spaces with Customized UniProt XML Files**; Joseph B Greer[1]; Ryan T Fellers[1]; Rich D Leduc[1]; Mick Greer[2]; David M Horn[3]; Kenneth R Durbin[1]; [1]*Proteinaceous, Evanston, IL;* [2]*Thermo Fisher Scientific, Austin, TX;* [3]*ThermoFisher Scientific, San Jose, CA*

WP 547   **Top-Down Proteomics of Myofilaments in Neonatal Swine Hearts throughout Development**; Timothy Aballo[1]; Ziqing Lin[1, 2]; Elizabeth Bayne[2]; Trisha Tucholski[2]; Wuqiang Zhu[3]; Meng Zhao[3]; Ahmed Mahmoud[1]; Jianyi Zhang[3]; Ying Ge[1, 2]; [1]*Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [3]*Department of Biomedical Engineering, University of Alabama at Birmingham, Birmingham, AL*

SMALL MOLECULES: QUANTITATIVE ANALYSIS II
WP 548-573

WP 548   **A simple and selective liquid chromatography-tandem mass spectrometric method for simultaneous determination of midazolam and 1-OH midazolam in human plasma**; Wuyi (charlie) Zha[1]; Xianglin Yuan[1]; Jinyuan Zhang[1]; Mike (qingtao) Huang[2]; Sudhakar Pai[2]; Luca Matassa[1]; Zhongping (john) Lin[1]; [1]*Frontage Laboratories Inc, Exton, PA;* [2]*Akros Pharma Inc., Princeton, NJ*

WP 549   **Impact of Sampling Rate and Transition Summing on Assay Variability for Triple Quadrupole Based Quantitative Analysis**; Wei Zeng[1]; Kevin P. Bateman[1]; [1]*Merck Research Laboratories, West Point, PA*

WP 550   **Development of a sensitive and high-throughput UPLC–MS/MS method for the quantification of 1-methylnicotinamide in human serum and urine**; Raymond Edward West Iii[1]; Thomas Nolin[1]; [1]*University of Pittsburgh, Pittsburgh, PA*

WP 551   **Development and Validation of an LC-MS/MS Method for the Quantitation of the Antiretroviral Elvitegravir Extracted from Human Hair**; Amanda P Schauer[1]; Craig Sykes[1]; Amanda Poliseno[1]; Heather MA Prince[1]; Angela DM Kashuba[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 552   **A Facile and Ultrasensitive Method for the Quantification of Monomethyl Fumarate (MMF) in Mouse Intestines, Blood, and Plasma Using LC-MS/MS**; Renmeng Liu[1]; Mingming Wang[1]; Deping Cheng[1]; [1]*Alliance Pharma, Inc., Malvern, PA*

WP 553   **Development of a high throughput Affinity Mass Spectrometry platform using Laser Diode Thermal Desorption ionization coupled to Mass Spectrometry (LDTD-MS)**; Aniruddha Sahasrabuddhe[1]; Dylan Oakley[1]; Kui Chen[1]; John Mccarter[1]; [1]*Amgen Inc., Thousand Oaks, CA*

WP 555   **Determination of Nitrosamine impurities in Losartan Potassium drug substance using Triple Quadrupole Liquid Chromatography Mass Spectrometry**; Chander Mani[1]; Saikat Banerjee[1]; [1]*Agilent Technologies, Haryana, India*

WP 556   **No Chiral Inversion for SEP-363856 in Humans by A Novel Chiral LC-MS/MS Analysis of Human Plasma from Clinical Trials**; Yu-Luan Chen[1]; Yao Shi[2]; Amber Lafayette[2]; Kenneth S. Koblan[1]; Gerald Galluppi[1]; [1]*Sunovion Pharmaceuticals, Inc., Marlborough, Massachusetts;* [2]*Covance Laboratories, Madison, WI*

WP 557   **Simultaneous Determination of Risperidone, Olanzapine, Aripiprazole, Amisulpride, Quetiapine, Haloperidol, Zuclopenthixol, and Fluphenazine (8-in-1) in Human Plasma by LC-MS/MS**; Yu-Luan Chen[1]; Junyi Yang[2]; Xiaonan Tang[2]; John (zhongping) Lin[1]; [1]*Sunovion Pharmaceuticals, Inc., Marlborough, Massachusetts;* [2]*Frontage Laboratories, Inc., Exton, PA*

WP 558   **Method Validation for the Determination of Methadone in Human Serum by Liquid Chromatography Coupled to Mass Spectrometry (LC/MS/MS)**; Amber Awad[1]; Ana Celia Grenier[1]; Lawrence J. Andrade[1]; [1]*Dominion Diagnostics, North Kingstown, RI*

WP 559   **High-Sensitivity Measurement of Estrogens without Derivatization in Human Serum Using EVOLUTE® EXPRESS ABN Prior to LC/MS-MS Analysis**; Mohamed Youssef[1]; M.rabie Al-Turkmani[2]; Petch Kaewsuya[2]; Suzanne Kamel-Mohamed[2]; Elena Gairloch[1]; [1]*Biotage, Charlotte, NC;* [2]*Labtech Diagnostics, Anderson, SC*

WP 560   **5-plex Mass Defect-based Isobaric Multiplex Reagents for Carbonyl-Containing Compound (mdSUGAR) Tags for Multiplex Quantification of N-glycans**; Xiaorong Lin[1, 2]; Miyang Li[3]; Yuanyuan Lin[1, 4]; Lingjun Li[1, 3]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222;* [2]*College of Food Science, South China Agricultural University, Guangzhou, China;* [3]*Department of Chemistry, University of*

Wisconsin-Madison, Madison, Wisconsin 53705-2222; [4]School of Pharmacy, Xi'an Jiaotong University, Xi'an, China

WP 561   **Analysis of Spatially Distinct Skin Sections by Laser Capture Microdissection and Microflow LC-MS/MS**; Jason Barricklow[1]; James Finley[1]; Lindsay Tomlinson[1]; Brett Hollingshead[1]; Colleen Doshna[1]; *[1]Pfizer, Groton, CT*

WP 562   **Populational Newborn Screening for Early Detection of Mucopolysaccharidoses by UPLC-MS/MS Using Urine Samples Collected on Filter Paper**; Iskren Menkovic[1]; Anne-Sophie Marchand[1]; Michel Boutin[1]; Christiane Auray-Blais[1]; *[1]Division of Medical Genetics, Department of Pediatrics, Faculty of Medicine & Health Sciences, Université de Sherbrooke, Centre de recherche-CHUS, CIUSSS de l'Estrie-CHUS, Sherbrooke, Quebec*

WP 563   **Identification and Quantitation of Nitrosamine impurities in various pharmaceutical API and drug substances**; Sandeep Choudhary[1]; Chandrasekar M[1]; Aman Sharma[1]; Manoj G Pillai[1]; *[1]Sciex, Gurugram, India*

WP 564   **Comprehensive identification and quantitation of Nitrosamine Impurities by HPLC-MS/MS** Jack Steed[1]; Jianru Stahl-Zeng[2]; Ferran Sanchez[2]; *[1]Sciex, Warrington, United Kingdom; [2]Sciex Germany GmbH, Darmstadt, Germany*

WP 565   **Development of Highly Sensitive Bioanalytical Methods For Peptide Based Therapeutics**; Xiaodong Zhu[1]; Jingguo Hou[1]; Karin Keller[1]; *[1]Worldwide Clinical Trials, Austin, TX*

WP 566   **Targeted Screening for >400 Prohibited Substances Using the Orbitrap Exploris 480**; Sophie Bromilow[1]; Elizabeth Walker[2]; Michael W. Senko[2]; Scott D Stanley[1]; *[1]University of Kentucky, Lexington, KY; [2]ThermoFisher Scientific, San Jose, CA*

WP 567   **Development of a cost-effective and highly selective bioanalytical method for the analysis of Montelukast in plasma using LC-MS/MS**; Prasanth Joseph[1]; Chidella Kartheek Srinivas[1]; Arun Kumar P[1]; Saikat Banerjee[1]; Samir Vyas[2]; *[1]Agilent Technologies, BENGALURU, India; [2]Agilent Technologies, Mumbai, India*

WP 568   **Quantitation of Multi Residues Antibiotics in Milk Using the SCIEX Triple Quad™ 3500 System**; Chandra Sekar[1]; Sabari Nathan[1]; Manoj G Pillai[1]; Lakshmanan D[1]; Jianru Stahl- Zeng[2]; *[1]Sciex, Gurugram, India; [2]Sciex Germany GmbH, Darmstadt, Germany*

WP 569   **LC/MS/MS Method development and validation of fosaprepitant (fAPT) and aprepitant (APT) in K3EDTA treated rat plasma**; Rachel Sun[1]; Hasantha Jayaratna[1]; Natasha Campbell[1]; Scott Clark[1]; *[1]Inotiv, West Lafayette, IN - Indiana*

WP 570   **Validated LC-MS/MS Assay for Quantitation of Venetoclax in Human K2EDTA Plasma**; Robert Clegg[1]; Ashton Hjerstedt[1]; Rachel Sun[1]; *[1]Inotiv, West Lafayette, Indiana*

WP 571   **Method Development for the separation and determination of cis-/trans-ceftibuten in human plasma by LC-MS/MS**; Jingguo Hou[1]; Xiaodong Zhu[1]; Karin Keller[1]; Shaolian Zhou[1]; *[1]Worldwide Clinical Trials, Austin, TX*

WP 572   **ELECTROSPRAY IONIZATION VERSUS ATMOSPHERIC PRESSURE SPRAY IONIZATION FOR BIOANALYSIS OF ACETYLCHOLINE FROM CEREBROSPINAL FLUIDS USING LIQUID CHROMATOGRAPHY–TANDEM MASS SPECTROMETRY**; Laszlo Prokai[1]; Vien Nguyen[1]; Daniel L. De La Cruz[1]; Katalin Prokai-Tatrai[1]; *[1]University of North Texas Health Science Center, Fort Worth, TX*

WP 573   **Rapid Quantitative Analysis of Fermentation Broth Samples to Assess Efficiency of Engineered Yeast Strain Turnover**; Rahul Baghla[1]; Rolf Kern[1]; Chang Liu[2]; Axel Besa[3]; Neil Walsh[4]; *[1]SCIEX, Redwood Shores, CA; [2]SCIEX, Concord, ontario; [3]Sciex Germany GmbH, Darmstadt, Germany; [4]Sciex, Warrington, United Kingdom*

SYSTEMS BIOLOGY
WP 574-586

WP 574   **Epigenetic Signatures that Regulate Caste Plasticity of Leafcutter Ants**; Michael Gilbert[1]; Balint Z Kacsoh[1]; Cristina M Brady[1]; Benjamin A. Garcia[1]; Shelley L Berger[1]; *[1]University of Pennsylvania, Philadelphia, PA*

WP 575   **Multi-omics identifies the role of RNA splicing dysfunction in Alzheimer's disease**; Xian Han[1, 2]; Ping-Chung Chen[1]; Junmin Peng[1]; *[1]St jude Children's research hospital, Memphis, TN; [2]University of Tennessee Health Science Center, Memphis, TN 38163*

WP 576   **Analytical Deconvolution and Characterization of Mixed Phenotypic Subpopulations in Wild-Type Salmonella**; Michelle Reid[1]; Alyson Hockenberry[2]; Nicola Zamboni[1]; *[1]Institute of Molecular Systems Biology, Department of Biology, ETH Zürich, Zürich, Switzerland; [2]Institute of Biogeochemistry and Pollutant Dynamics, Department of Environmental Microbiology, ETH Zürich, Dübendorf, Switzerland*

WP 577   **Dynamic metabolic network modeling of a cytokine-induced mammalian cell cycle using time-course metabolomics and proteomics**; Ho-Joon Lee[1]; Fangzhou Shen[2]; Sriram Chandrasekaran[3]; *[1]Yale University, New Haven, CT; [2]University of Michigan, Ann Arbor, MI; [3]University of Michigan, Ann Arbor*

WP 578   **R2-P2 rapid-robotic phosphoproteomics enables multidimensional cell signaling studies**; Mario Leutert[1]; Ricard A Rodriguez-Mias[1]; Noelle K Fukuda[1]; Judit Villen[1]; *[1]Department of Genome Sciences, University of Washington, Seattle, WA*

WP 579   **NanoLC-MS Based Discovery Proteomic Analysis of the Frog Inner Ear**; Aparna B. Baxi[1, 2]; Peter Nemes[3, 4];
Sally A. Moody[3]; [1]*The George Washington University, Washington Dc, DC;* [2]*University of Maryland College Park,
College Park, MD;* [3]*George Washington University, Washington, DC;* [4]*University of Maryland, College Park, MD*

WP 580   **Integrating quantitative proteomic and metabolomic measurements to optimize microbial cellular extract
preparation for enhanced cell-free protein synthesis**; Payal Chirania[1, 2]; Richard J. Giannone[1, 2]; Nancy L.
Engle[1]; Grant A. Rybnicky[3]; Blake J. Rasor[3]; Timothy J. Tschaplinski[1]; Michael C. Jewett[3]; Robert L. Hettich[1, 2];
[1]*Oak Ridge National Laboratory (ORNL), Oak Ridge, TN;* [2]*University of Tennessee Knoxville, Knoxville, TN;*
[3]*Northwestern University, Evanston, IL*

WP 581   **Untargeted systems biology approach to identify proteomic biomarkers of radiation-induced injury**;
Weiliang Huang[1]; Ann M Farese[1]; Thomas J MacVittie[1]; Maureen Kane[2]; [1]*University of Maryland Balitmore,
Baltimore, MD;* [2]*Universityof Maryland, Baltimore, Baltimore, MD*

WP 582   **Quantitative top down proteoform analysis of EZH2 inhibition in renal medullary carcinoma cells reveals
compensatory mechanism for combinatorial therapy**; Nikit Venishetty[1, 2]; Tao Wang[2]; Karl F. Poncha[2];
Matthew V. Holt[2]; Nicolas L. Young[2]; [1]*Rice University, Houston, Texas;* [2]*Baylor College of Medicine, Houston,
Texas*

WP 583   **Identifying HDAC3 as a delactylase using quantitative proteomics**; Di Zhang[1]; Lu Yang[1]; Jinjun Gao[2];
Yingming Zhao[1]; [1]*Ben May Department for Cancer Research, The University of Chicago, Chicago, Illinois;*
[2]*University of Chicago, Chicago, IL*

WP 584   **MOTA: Network-Based Method for Multi-Omic Integrative Analysis**; Ziling Fan[1]; Habtom Ressom[1]; Yuan
Zhou[1]; [1]*Georgetown University, Washington, DC*

WP 585   **A New Microflow LC-MS Platform for Simultaneous Multiomics Analysis**; Daojing Wang[1]; Kai Szeto[1]; Weimin
Ni[1]; Pan Mao[1]; [1]*Newomics Inc., Berkeley, CA*

WP 586   **Protein-protein interaction-guided functional enrichment analysis for mass spectrometry-based
quantitative proteomics**; Rachel Nadeau[1]; Anastasiia Byvsheva[1]; Mathieu Lavallée-Adam[1]; [1]*University of
Ottawa, Ottawa, ON*

BIOMARKERS: DISCOVERY III
ThP 001-015

ThP 001 **Multiplexed Quantitative Proteomics Provides Mechanistic Cues for Malaria Severity and Complexity**; Vipin Kumar[1]; Shalini Aggarwal[1]; Deeptarup Biswas[1]; Sanjeev V Sabnis[1]; Arunansu Talukdar[2]; Swati Patankar[1]; Sanjeeva Srivastava[1]; [1]*Indian Institute of Technology, Bombay, Mumbai, India;* [2]*Medical College Kolkata, Kolkata, India*

ThP 002 **Spatially-Resolved Proteomics Guided by MALDI MS Imaging and Integrated to Clinical Data Leads to Glioblastoma Patients Stratification for Precision Medicine**; Lauranne Drelich[1]; Marie Duhamel[1]; Maxence Wisztorski[1]; Patrick Devos[2]; Fabienne Escande[3]; Claude-Alain Maurage[3]; Emilie Le Rhun[1, 4]; Isabelle Fournier[1]; Michel Salzet[1]; [1]*Université de Lille, Inserm, U1192, Laboratoire Protéomique, Réponse Inflammatoire et Spectrométrie de Masse (PRISM), Bâtiment SN3, 1er étage,, Villeneuve D'ascq Cedex, France;* [2]*Univ. Lille, CHU Lille, EA 2694 - Santé Publique: Épidémiologie et Qualité des Soins, Lille, France;* [3]*Univ. Lille, CHU Lille, Pôle Pathologie Biologique, Service Anatomie Pathologique, Lille, France;* [4]*Univ. Lille, CHU Lille , Neuro-Oncology, Neurology Department, Roger Salengro Hospital, Rue Emile Laine, Lille, France*

ThP 003 **Monitoring the differentiation process of human induced pluripotent stem cells (hiPSCs) to cerebral cortical neurons by LC-MS/MS media analysis**; Nobuhiko Kondo[1]; Keiko Ishibe[1]; Takashi Suzuki[1]; Kenichi Toyoda[1]; Hirotaka Kuroda[1]; Toru Ezure[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

ThP 004 **Multiple-Reaction Monitoring (MRM)-Profiling Reveals Distinct Lipid and Metabolite Profiles in Microglia with Amyloid Beta Exposure**; Priya Prakash[1]; Jonathan A. Fine[1]; Elizabeth A. Thayer[1]; Christina R. Ferreira[1]; Gaurav Chopra[1]; [1]*Purdue University, West Lafayette, IN*

ThP 005 **FAIMS Dramatically Increases Proteome Coverage for Top-Down Discovery and Biomarker Experiments**; Robert V Gerbasi[1]; Rafael D Melani[2]; Sue Abbatiello[3]; Romain Huguet[4]; Michael W. Bedford[4]; Scott Peterman[4]; John P Mcgee[2]; Philip D. Comption[2]; Paul Thomas[2]; Joshua Levitsky[5]; Neil L Kelleher[2]; [1]*Northwestern University, Evanston, IL;* [2]*Northwestern University, Evanston, IL/60208;* [3]*Northeastern University, Boston, MA;* [4]*Thermo Fisher Scientific, San Jose, California;* [5]*Northwestern University, Chicago, IL*

ThP 006 **Differential integration of transcriptome and proteome to explore age-specific changes in exosomes**; Sandip Kumar Patel[1]; Jonathan Levi[1]; Roland Bruderer[2]; Francesco Neri[1]; Nathan Basisty[1]; Lukas Reiter[2]; Judith Campisi[1, 3]; Birgit Schilling[1]; [1]*The Buck Institute for Research on Aging, Novato, CA;* [2]*Biognosys AG, Schlieren, Switzerland;* [3]*Lawrence Berkeley Laboratory, University of California, Berkeley, California*

ThP 007 **Phosphoproteomics revealed activation of ATM signaling pathway in lenalidomide resistant multiple myeloma**; Santosh Renuse[1, 2]; Yuan Xiao Zhu[3]; Dong-Gi Mun[1]; Anil K Madugundu[1]; Kiran K Mangalaparthi[1]; Chang-Xin Shi[3]; A. Keith Stewart[2, 3]; Akhilesh Pandey[1, 2]; [1]*Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN;* [2]*Center for Individualized Medicine, Mayo Clinic, Rochester, MN;* [3]*Division of Hematology and Oncology, Mayo Clinic, Scottsdale, AZ*

ThP 008 **Multi-Omic Profiling of Cerebrospinal Fluid from Alzheimer's Disease Patients**; Whitaker Cohn[1]; Erdim Sertoglu[1]; Harry V Vinters[1]; Kym F Faull[1]; Varghese John[1]; Julian P Whitelegge[1]; [1]*University of California, Los Angeles, Los Angeles, CA*

ThP 009 **Differential Metabolomics Profile of Human Blastocysts: Can It Be a Potential Predictor of Viability of Transferred-Embryos for Prospective Pregnancy Outcome**; Vani V[1]; Saikrshna S.b[2]; Rajesh Babu D[3]; Venketesh S[4]; Vasan S.s[5]; Adiga S.k.[6]; Varsha S.r.[7]; Sachdeva G.[8]; Seshagiri P.b.[9]; [1]*Indian Institute of Science, Department of Molecular Reproduction, Development and Genetics, Sir CV Raman Road, Bangalore, India;* [2]*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning, India, Puttaparthi, India;* [3]*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning,, Puttaparthi,, India;* [4]*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning, India, Puttaparthi,, India;* [5]*Manipal Ankur Andrology & Reproductive Services, Bangalore,, India;* [6]*4Kasturba Medical College, Department of Clinical Embryology, Manipal,, India;* [7]*Advanced Fertility Centre,, Bangalore, India;* [8]*National Institute for Research in Reproductive Health, Mumbai, India;* [9]*Indian Institute of Science, Department of Molecular Reproduction, Development and Genetics, Sir CV Raman Road, Bangalore, India*

ThP 010 **GC-MS analysis of albumin synthesis to assess the effect of novel feed compounds on broiler chickens**; Jorge Peinado-Izaguerri[1, 2]; Francesca Riva[1, 3]; Alexandra C. Small[1]; Mark Mclaughlin[1]; Dorothy Mckeegan[1]; Maureen Bain[1]; Mangesh Bhide[2]; Tom Preston[1]; [1]*University of Glasgow, Glasgow, UK, Glasgow, UK, United Kingdom;* [2]*University of Veterinary Medicine and Pharmacy in Kosice, Kosice, Slovakia;* [3]*University of Zagreb, Zagreb, Croatia*

ThP 011 **Machine Learning Predicts Renal Cell Carcinoma Status from Urine Using Multiplatform Metabolomics**; Olatomiwa O Bifarin[1, 2]; David A Gaul[3]; Rebecca S Arnold[4]; John A. Petros[4, 5]; Facundo M. Fernandez[3]; Arthur S. Edison[1, 2]; [1]*Department of Biochemistry and Molecular Biology, University of Georgia, Athens, 30602;* [2]*Complex Carbohydrate Research Center, University of Georgia, Athens, 30602;* [3]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, 30332;* [4]*Department of Urology, Emory University, Atlanta, 30342;* [5]*Atlanta VA Medical Center, Atlanta, 30033*

ThP 012 **Proteograph, a novel multi-nanoparticle platform, enables rapid and deep proteomics profiling, significantly improving coverage, throughput, and scalability versus existing methods**; John E. Blume[1]; Shadi Ferdosi[1]; Daniel Hornburg[1]; Matthew E. K. Chang[2]; Philip C. M. Ma[1]; Omid C. Farokhzad[1]; Mark R. Flory[2]; Patrick A. Everley[1]; *[1]Seer, Inc., Redwood City, CA; [2]Cancer Early Detection Advanced Research Center (CEDAR), Knight Cancer Institute (KCI), Oregon Health and Science University (OHSU), Portland, OR*

ThP 013 **Proteomics analysis of cellular response in NIH-3T3 cells cultured in different stress conditions using three-dimensional collagen hydrogels**; Matthew W Turner[1]; Stephanie Frahs[1]; Xinzhu Pu[1]; Laura Bond[1]; Trevor Lujan[1]; Cindy Keller-Peck[1]; Julia Thom Oxford[1]; *[1]Boise State University, Boise, ID*

ThP 014 **Cathepsin B Dependent Cleavage Product of Serum Amyloid A1 Identifies Patients with Chemotherapy-Related Cardiotoxicity**; Jia Fan[1]; Bo Ning[1]; *[1]Tulane University, New Orleans, LA*

ThP 015 **Metabolomics study reveal the protective effect of Apigenin on APAP-induced liver injury**; Cheng Hu[1]; Yiqun Jia[1]; *[1]Shanghai University of Traditional Chinese Medicine, Shanghai, China*

BIOMARKERS: QUANTITATIVE ANALYSIS III
ThP 016-029

ThP 016 **Building Bridges between Immuno-Oncology and Molecular Pathology: Development of a Quantitative Immuno-MRM Assay for the PD-1/PD-L1 Axis**; Vincent Lacasse[1, 2]; Vincent R. Richard[1]; Georgia Mitsa[1]; Oliver Poetz[3]; René Zahedi[1]; Alan Spatz[4, 5]; Christoph H. Borchers[1, 4, 6]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [2]Department of Pathology, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [3]Signatope GmbH, Reutlingen, Germany; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [5]Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; [6]Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

ThP 017 **High-throughput Proteomics Approach for Systematically Profiling Phosphotyrosine Signaling Complexes**; Qian Kong; *Hong Kong Baptist University, Shenzhen, China*

ThP 018 **Quantitative Analysis of Clinical Proteome in Nipple Discharge by Nano LC-Nano-ESI-SRM-MS Using Stable Isotope-labeled Iodoacetanilide**; Sadamu Kurono[1]; Satomi Niwayama[2]; *[1]FUJIFILM Wako Pure Chemical Industries, Ltd., Osaka, Japan; [2]Muroran Institute of Technology, Muroran, Japan*

ThP 019 **Immunoaffinity LC/MS for the Quantitation of Mouse PD1, PD-L1 in Tumor for Drug/Target Characterization Study**; Yongxin Zhu[1]; Petia Shipkova[1]; Jacob Zalaznick[1]; Bogdan Sleczka[1]; Matthew Mazur[1]; Zheng Yang[1]; Karen Parrish[1]; Jesse Swanson[1]; Anwar Murtaza[1]; Timothy Olah[1]; *[1]Bristol-Myers Squibb Company, Princeton, NJ*

ThP 020 **Rapid High-Throughput Profiling and Quantitation of Sialic Acids in Biotherapeutics**; Anna Fong[1]; Ace G. Galermo[1]; John Yan[1]; Tom Rice[1]; Aled Jones[1]; Archana Datt[1]; Hamutal Bonen[1]; Gregory Staples[1, 2]; Ted Haxo[1]; *[1]Agilent Technologies, Hayward, CA; [2]Agilent Technologies, Santa Clara, CA*

ThP 021 **Novel target LC-MS methods to detect protein biomarkerin human serum extracellular vesicles**; Fengping Li[1]; Lindsay King[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA*

ThP 022 **Isolation and Determination of Cell Surface, Intracellular, ExtracellularPD-1 using Cell Surface Labeling**; Huidong Gu[1]; Marissa Demichele[1]; Yue Zhao[1]; Brian Schmidt[1]; Yan J Zhang[1]; Renuka Pillutla[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb Company, Princeton, NJ*

ThP 023 **Quantification of dermatan sulfate, chondroitin sulfate and heparan sulfate in tissues from mutant mice with mucopolysaccharidosis type VI using UPLC-MS/MS**; Haoyue Zhang[1]; Mireille Tallandier[2]; Olivier Lacombe[2]; Eugeni Entchev[2]; James Beasley[1]; Ashlee R Stiles[1]; Sarah P Young[1]; *[1]Duke University Health System, Durham, NC; [2]Inventiva Pharma, Dijon, France*

ThP 024 **A Novel, Fast, Accurate, and Robust Hybrid LC-MS/MS Method for Quantification of Hemoglobin A1c: Bioanalytical Method Development, Optimization, and Validation**; Shuyu Hou[1]; Xiaolei Liu[1]; Tian-Sheng Lu[1]; Guangchun Zhou[1]; *[1]Medpace, Cincinnati, OH*

ThP 025 **Developing molecular-specific biomarker assays for IgA vasculitis with nephritis**; Alyssa L. Hansen[1]; Ellenore P. Craine[1]; Audra A. Hargett[1]; Stacy D. Hall[1]; Bruce A. Julian[1]; Jan Novak[1]; Matthew B. Renfrow[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

ThP 026 **Quantification of creatinine in urine samples by High-Throughput Screening (HTS) using LDTD-MS/MS**; Francis Briere[1]; Pier-Luc Plante[1]; Jean Lacoursière[2]; Serge Auger[2]; Jacques Corbeil[1]; Pierre Picard[2]; *[1]Université Laval, Québec, QC; [2]Phytronix Technologies, Quebec, QC*

ThP 027 **Development of a PD Biomarker assay to monitor glutaminase inhibition in peripheral blood mononuclear cells after treatment with glutaminase inhibitors**; Yongying Jiang[1]; Jihai Pang[1]; Nakia Spencer[1]; Quanyun Xu[1]; Anastasia Lopez[1]; Thomas Quill[1]; Jennifer Linares[1]; Angela Harris[1]; Jeffery Kovacs[1]; Timothy Heffernan[1]; Kang Le[1]; Michael Soth[1]; Philip Jones[1]; *[1]MD Anderson Cancer Center, Houston, TX*

ThP 028 **Fast Accurate Quantitative Bioanalysis of sBCMA in Plasma under GLP: Comparison of AQUA, MIRM-ISCC and Conventional External Calibration Curve Approaches**; Laurence Mayrand-Provencher; *Caprion Biosciences, Montreal, QC*

ThP 029 **LC-high resolution mass spectrometry for quantitative assay of advanced glycation end-products in plasma**; Hye Kyong Kweon[1]; Edwin Miranda[2]; Jacob M. Haus[2]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]School of Kinesiology, University of Michigan, Ann Arbor, MI*

CLINICAL ANALYSIS III
ThP 030-051

ThP 030 **A Microsampling Assay for the Quantitation of Vancomycin in Human Whole Blood**; Christina Vedar[1]; Ganesh Moorthy[1]; Kevin J Downes[1]; Athena F Zuppa[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA*

ThP 031 **Determination of   25(OH)VD3 derivatives in LC-MS with special reversed-phase chromatographic columns**; Haijun An[1]; Qiqi Tu[1]; *[1]Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China*

ThP 032 **A Comparative proteomics study of mental disorders: Schizophrenia and Bipolar Disorder**; Ramesh Rajendran[1]; Aparna Sundaresh[2]; Vir Singh Negi[2]; Vijayalakshmi M.a.[1]; Kamalanathan A.s.[1]; *[1]Centre for BioSeparation Technology, Vellore Institute of Technology, Vellore, India; [2]Department of Clinical Immunology, JIPMER, Puducherry, India*

ThP 033 **Quantitative On-Site Harm Reduction Drug Checking in the Opioid Overdose Crisis using Paper Spray Mass Spectrometry**; Scott A. Borden[1, 2]; Armin Saatchi[1]; Gregory W. Vandergrift[1, 2]; Nicole M. Esligar[3]; Samuel Tobias[3]; Mark Lysyshyn[4, 5]; Jan Palaty[6]; Erik T. Krogh[1, 2]; Christopher G. Gill[1, 2, 7, 8]; *[1]Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC; [2]University of Victoria, Victoria, British Columbia; [3]BC Centre on Substance Use, Vancouver, BC; [4]Vancouver Coastal Health Authority, Vancouver, BC; [5]University of British Columbia, Vancouver, BC; [6]Lifelabs Medical Laboratories, Burnaby, BC; [7]Simon Fraser University, Burnaby, BC; [8]University of Washington, Seattle, WA*

ThP 034 **Exemplary performance data of a Triple Quadrupole Mass Spectrometer in a simulated clinical LDT workflow**; Byungchul Cha[1]; Mindy Gao[1]; Kristine Van Natta[1]; Terry Olney[1]; Maurino Flora[1]; John Glazier[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 035 **Simultaneous determination of fat-soluble vitamins A, D, E and K in human serum using LC-MS/MS with SPE pretreatment**; Xiaoli Ma[1]; Qianqian Li[1]; Wenjing Liu[1]; Zhengwei Jia[1]; *[1]waters cooperation, Shanghai, China*

ThP 036 **Cost effective and rapid method for simultaneous determination of vitamin B12, 25-Hydroxyvitamin D2 and D3 from plasma using LC-MS/MS**; Bhaumik Trivedi[1]; Shailesh Damale[1]; Shailendra anil Rane[1]; Deepti Bhandarkar[1]; Purushottam Sutar[1]; Anant Lohar[1]; Ashutosh Shelar[1]; Navin Devadiga[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd, Mumbai, India*

ThP 038 **Control strategy for the matrix effect for actual study samples in regulated clinical analysis**; Jinhui Zhang[1]; Arindam Dasgupta[1]; Ruben Ayala[1]; Jianghong Gu[1]; Charles Bonapace[1]; Sean Kassim[1]; Patrick Faustino[1]; *[1]FDA, Silver Spring, MD*

ThP 039 **Evaluation of a rapid LC-MS/MS method to measure simultaneously IDUA and IDS enzymes activities in dried blood spots**; Misa Tanaka[1]; Tsubasa Oguni[2]; Yoshitomo Notsu[2]; Tetsuo Iida[3]; Takanari Hattori[4]; Jun Watanabe[4]; Hironori Kobayashi[5]; *[1]MS specialite, Yokohama, Japan; [2]Clinical Laboratory Division, Shimane University Faculty of Medicine, Izumo, Japan; [3]Shimadzu Corporation, Global Application Development Center, Kyoto, Japan; [4]Shimadzu Corporation, MS Business Unit, Kyoto, Japan; [5]Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan*

ThP 040 **Proteomic evaluation of ALA induced fluorescence in Glioblastoma to understand biological heterogeneity**; Saicharan Ghantasala[1]; Deeptarup Biswas[1]; Aliasgar Moiyadi[2]; Sridhar Epari[3]; Sanjeeva Srivastava[4]; *[1]Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, India; [2]Division of Neurosurgery, Department of Surgical Oncology, Tata Memorial Centre, Homi Bhabha National University, Mumbai, India; [3]Department of Surgical Pathology, Tata Memorial Centre, Homi Bhabha National University, Mumbai, India; [4]IIT Bombay, Mumbai, India*

ThP 041 **A rapid and highly sensitive LC-MS/MS method for bioanalysis of biotin in human plasma**; Peiling Hou[1]; Djohan Kesuma[1]; Jie Xing[1]; *[1]Shimadzu (Asia Pacific), Singapore, Singapore*

ThP 042 **Development and validation of a dried blood spot LC-MS/MS method for indomethacin analysis**; Whitney Nolte[1]; Kim Gibson[1]; Allison Scott[1]; Tamorah Lewis[1]; *[1]Children's Mercy Hospital, Kansas City, Kansas City, MO*

ThP 043 **A High-Throughput Integrated HRAM-MS Method Enables IGF-1 Quantification, Targeted Variants Monitoring, and Untargeted Variants Screening in a Single Injection**; Yu Zhou[1]; Xiaolei Xie[1]; Kristine Van Natta[1]; Bradley Hart[1]; Shen Luan[1]; Debadeep Bhattacharyya[1]; *[1]Thermo Fisher Scientific, San Jose, California*

ThP 044 **Development and Implementation of an LC/MRM-MS Assay for a Panel of Antibiotics/Antifungals in Intensive Care Unit Clinical Settings**; Evgeniy V. Petrotchenko[1]; Shaun Eintracht[2]; Christoph H. Borchers[1, 3, 4];

[1]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [2]*Department of Diagnostic Medicine, Jewish General Hospital, Montreal, Canada, Montreal, QC;* [3]*Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC;* [4]*Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

ThP 045   **The Simultaneous Quantitation of Five Tri-azole Anti-fungal Agents from Plasma Utilizing Paper Spray-Mass Spectrometry**; Lindsey M Kirkpatrick[1]; Christine L Skaggs[2]; Greta J Ren[2]; El Taher M Elgierari[3]; Lillian R Strumer[4]; Run Z Shi[4]; Nicholas E. Manicke[2, 5]; [1]*Indiana University School of Medicine, Pediatric Infectious Disease, Indianapolis, IN;* [2]*Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN;* [3]*Stanford Health Care, Palo Alto, CA;* [4]*Department of Pathology, Stanford University School of Medicine, Stanford, CA;* [5]*Forensics and Investigative Sciences, Indiana University-Purdue University Indianapolis, Indianapolis, IN*

ThP 047   **Is a low blood somatostatin (SST) concentration responsible for migraine with aura? An LC-MS/MS study**; Ramneek Kaur[1]; Dr. David Harman[1]; Dr. David A Mahns[1]; [1]*Western Sydney University, Campbelltown, Australia*

ThP 048   **Targeted serum glycoprotein profiling and quantification by LC-MS/MS for detection of ovarian cancer**; Gege Xu[1]; Daniel Serie[1]; Ling Shen[1]; Padraig Buckley[1]; Maurice Wong[1]; Prasanna Ramachandran[1]; Rachel Rice[1]; Carlito Lebrilla[1]; Klaus Lindpaintner[1]; Hui Xu[1]; [1]*InterVenn Biosciences, South San Francisco, CA*

ThP 051   **High Resolution UHPLC-MS/MS Identification and Characterization of Superwarfarin Metabolites in Human Blood**; Daniel Nosal[1]; Douglas L Feinstein[2]; Richard B. Van Breemen[1]; [1]*Oregon State University - Linus Pauling Institute, Corvallis, OR;* [2]*University of Illinois at Chicago - Department of Anesthesiology, Chicago, IL*

CORPORATE POSTERS IV
ThP 052-054

ThP 052   **Bruker at ASMS 2020: MALDI II for dramatic sensitivity improvements in SpatialOMx workflows, Bruker Daltonics**

ThP 053   **Analytical Intelligence in the Digital Age of Mass Spectrometry, Shimadzu Scientific Instruments**

ThP 054   **Orbitrap Exploris Mass Spectrometry, Thermo Fisher Scientific**

DRUG METABOLISM: QUALITATIVE ANALYSIS
ThP 056-067

ThP 056   **Piperazine in a Tyrosine Kinase Inhibitor, Should We Throw the Red Flag? An In silico and Practical Bioactivation Approach.**; Thamer Alsubi[1]; Adnan A Kadi[1]; Hany W Darwish[1]; [1]*King Saud University, Riyadh, Saudi Arabia*

ThP 057   **Workflow automation for lipidated peptide metabolite profiling**; Tatiana Radchenko[1]; Jon Griffin[2]; Fabien Fontaine[1]; Ismael Zamora[1, 3]; [1]*Lead Molecular Design S.L., Sant Cugat de Valles, Spain;* [2]*Zealand Pharma A/S, Copenhagen, Denmark;* [3]*Molecular Discovery, Ltd., Borehamwood, United Kingdom*

ThP 058   **Biosynthesis and Structural Elucidation of Drug Metabolites by LC-MS and LC-SPE-NMR**; Pingrong Liu[1]; Dongyue Xin[1]; Nina Gonnella[1]; Mitchell Taub[1]; Aaron Teitelbaum[1]; [1]*Boehringer Ingelheim Pharm. Inc., Ridgefield, CT*

ThP 059   **Rapid and sensitive ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS) determination of nicotine and its metabolites in rat plasma and tissues.**; Estatira Sepehr[1]; Qiangen Wu[1]; Matthew S Bryant[1]; [1]*National Center for Toxicological Research, FDA, Jefferson, AR*

ThP 060   **Development and Validation of a LC-MS/MS Method for the Quantitation of Tenofovir Diphosphate in Dog PBMCs**; Jingduan Chi[1]; Fumin Li[1]; Dennis Kraus[1]; Yonghua Ling[1]; Shane Roller[2]; [1]*PPD Inc, Madison, WI;* [2]*2 Intarcia Therapeutics, Inc. Boston, MA, Boston, MA*

ThP 061   **Clinical analysis of creatinine reduction in bone marrow transplants induced by four immunosuppressants**; Wang Lei; *Beijing Lu Daopei Institute of Hematology, Beijing, China*

ThP 062   **Investigation of LC-ESI-MS/MS method in biological samples for quantitative analysis of metformin carrying biguanide derivative features**; Jianmei Wang[1]; Kiran Chaudhari[1]; Yong Xu[1]; Ali Winters[1]; Xiaowei Dong[1]; Ran Liu[1]; Shaohua Yang[1]; [1]*University of North Texas Health Science Center, Fort Worth, Texas*

ThP 063   **Quantitation of Nucleoside and Phosphates Anabolites by Indirect Quantitation in Human Dried Blood Using Volumetric Absorptive Microsampling (VAMS)**; Cynthia M. Chavez-Eng[1]; Ryan Lutz[1]; Bing Lu[1]; Kerry Fillgrove[1]; Melanie Anderson[1]; Dina Goykhman[1]; Eric Woolf[1]; [1]*Merck & Co., West Point, PA*

ThP 064   **Identification and Quantification of the Metabolites of Peptide Conjugated Phosphorodiamidate Morpholino Oligomer (PPMO-A) in Human Plasma Using LC-MS/MS**; Zhiling Zhang[1]; Jianbo Zhang[2]; Erhu Lu[1]; Zhongping (john) Lin[1]; John Hadcock[2]; [1]*Frontage Laboratories, Inc., Exton, PA;* [2]*Sarepta Therapeutics, Cambridge, MA*

ThP 065   **Application of Orbitrap ID-X Tribrid Mass Spectrometer for Metabolite Profiling**; Ron Aoyama[1]; Kate Comstock[2]; [1]*Gilead Sciences Inc., Foster City, California;* [2]*Thermo Fisher Scientific, San Jose, CA*

ThP 066   **NAFLD/NASH: Toward biologically-relevant and robust preclinical models for a successful selection of your drug clinical candidate**; Rima Ait Belkacem[1]; Micheline Kergoat[2]; Alice Dufour[1]; Fawzia Mouveaux[2]; Sophie Raynal[2]; Lauranne Poncelet[1]; Laurent Benel[1]; Fabien Pamelard[1]; Sandrine Durand[2]; Armel Nijman[2]; Anthony Dessaux[1]; David Bonnel[1]; Valérie Autier[2]; Jonathan Stauber[3]; [1]*ImaBiotech, Loos, France;* [2]*Metabrain, Maisons-Alfort, France;* [3]*ImaBiotech, Billerica, Massachusetts*

ThP 067   **Quantitation of Contraceptive Hormones with Co-administered Antiretroviral Drugs in Human Plasma by LC-MS/MS**; Jeffrey Jeppson[1]; Lee Winchester[1]; Kayla Campbell[1]; Timothy Mykris[1]; [1]*UNMC, Omaha, NE*

ENVIRONMENTAL: GENERAL II
ThP 068-081

ThP 068   **Metabolomic analysis of effects of copper oxide nanoparticles and microparticles on microalga Chlorella vulgaris**; Lei Wang[1]; Xulei Huang[1]; Anna Karen Carrasco Laserna[1]; Sam Li[1]; [1]*National University of Singapore, Singapore, Singapore*

ThP 069   **Strategies for homologue series detection – Investigating the fate of small water-soluble polymeric substances in a waste water treatment plant**; Teresa Mairinger[1, 2]; Martin Loos[3]; Juliane Hollender[1, 4]; [1]*EAWAG, Duebendorf, Switzerland;* [2]*University of Natural Resources and Life Sciences-BOKU Vienna, Vienna, Austria;* [3]*envibee GmbH, Zurich, Switzerland;* [4]*ETH Zurich, Zurich, Switzerland*

ThP 070   **Detection of volatile compounds emitted by bed bugs (Cimex lectularius L.) using selected-ion flow-tube mass spectrometry (SIFT-MS)**; Jesse L. Balcer[1]; Neil A. Spomer[1]; Aaron R. Ashbrook[2]; Mary E. Rushton[1]; Jeffrey R. Gilbert[1]; Ameya D. Gondhalekar[2]; [1]*Corteva Agriscience, Indianapolis, IN;* [2]*Purdue University, West Lafayette, IN*

ThP 071   **Quantitative Determination of Per- and Polyfluoroalkyl Substances in Various Landfill Soils Using Ultra High-Pressure Liquid Chromatography/Tandem Mass Spectrometry (UHPLC-MS/MS)**; Atiye Ahmadireskety[1]; Bianca F Da Silva[2]; Richard A. Yost[1]; John A. Bowden[2]; [1]*Chemistry Department, University of Florida, Gainesville, Florida;* [2]*College of Veterinary Medicine, Department of Physiological Sciences, University of Florida, Gainesville, Florida*

ThP 072   **Analysis of PFAS compounds in Fish Tissue Using Offline Supercritical Fluid Extraction and LC-MS/MS**; William Hedgepeth[1]; Yuka Fujito[1]; Ruth Marfil-Vega[1]; Logan Miller[1]; [1]*Shimadzu Scientific Instruments, Inc, Columbia, MD*

ThP 073   **Integrated metabolomics and lipidomics approach reveal dramatic polyunsaturated lysoglycerophospholipids accumulation in human lung fibroblasts exposed to fine particulate matter**; Jong Cheol Shon[1]; Young Sang Kwon[1]; Hee-Jung Shim[1]; Min-Chul Shin[1]; Sung-Min Lee[1]; Jong-Hwan Kim[1]; Jong-Su Seo[1]; [1]*Korea Institute of Toxicology, Munsan-eup, Jinju, South Korea*

ThP 074   **Photolysis of Emerging Contaminants absorbed to Different plastics: Role of Surface Area**; Xiolmara Martinez[1]; Daryl Giblin[2]; Nicolas Jozefowski[1]; Michael L. Gross[2]; M. Paul Chiarelli[1]; [1]*Loyola University, Chicago, IL;* [2]*Washington University in St.Louis, St.Louis, Missouri*

ThP 075   **Metabolomics and lipidomics demonstrate two genetically similar lysogenic bacteria influence host metabolism based on growth substrate**; Katarina A. Jones[1]; Jonelle T. R. Basso[2]; Kaylee R. Jacobs[2]; Courtney J. Christopher[1]; Haley B. Fielland[1]; Alison Buchan[2]; Shawn R. Campagna[1, 3]; [1]*Department of Chemistry, University of Tennessee Knoxville, Knoxville, Tennessee;* [2]*Department of Microbiology, University of Tennessee Knoxville, Knoxville, Tennessee;* [3]*Biological and Small Molecule Mass Spectrometry Core, University of Tennessee Knoxville, Knoxville, Tennessee*

ThP 076   **Integrated Instrumental Approach for Characterization of Adsorbed Carcinogens and Heavy Metals on Firefighter Gear**; Drew I Stolpman[1]; Allyson Cliet[1]; Shubhneet Warar[1]; Amaan Allan[1]; Debra Harris[1]; Touradj Solouki[1]; [1]*Baylor University, Waco, TX*

ThP 078   **Using machine-learning approaches and multivariate statistics to understand driving environmental forces in a large microbial marine metaproteome**; Jaclyn Saunders[1]; Matthew Mcilvin[1]; Dawn Moran[1]; Noelle Held[1, 2]; Chris Dupont[3]; Alyson E. Santoro[4]; Mak Saito[1]; [1]*Woods Hole Oceanographic Institution, Woods Hole, MA;* [2]*Massachusetts Institute of Technology, Cambridge, MA;* [3]*J. Craig Venter Institute, Rockville, Maryland;* [4]*University of California Santa Barbara, Santa Barbara, CA*

ThP 079   **Evaluating desalination wastewaters as a source of disinfection by-products in aquatic ecosystems**; Danielle Westerman[1]; Leanne Powers[2]; Michael Gonsior[2]; Susan D. Richardson[1]; [1]*University of South Carolina, Columbia, SC;* [2]*University of Maryland Center for Environmental Science, Cambridge, MD*

ThP 080   **Biodegradation pathway of Anthraquinone dyes by a Novel Laccase from Trametes hirsute D7 fungus**; Rafiqul Alam[1]; Fenny Clara Ardiati[2]; Nissa Nurfajrin[2]; Dede Heri Yuli Yanto[2]; Sunghwan Kim[1, 3]; [1]*Department of*

Chemistry, Kyungpook National University, Daegu, South Korea; [2]Research Center for Biomaterials, Indonesian Institute of Sciences (LIPI), Bogor, Indonesia; [3]Green-Nano materials Research Center, Daegu, South Korea

ThP 081   **Analysis of Per-and Polyfluoroalkyl Substances (PFAS) Specified in EPA M533 Using the Triple Quadrupole LCMSMS**; Brahm Prakash[1]; Christopher T. Gilles[2]; Ruth Mafil-Vega[2]; William Lipps[2]; [1]*Shimadzu Scientific Instruments, Inc., Columbia, MD; [2]Shimadzu Scientific Instruments, Columbia, MD*

ENVIRONMENTAL: PHARMACEUTICALS AND PESTICIDES
ThP 082-098

ThP 082   **Towards Single System for Total Water Analysis. LC-MS/MS screening of 325 PPCP Contaminants in Tap and Surface Water**; Aurore Jaffuel[1]; Mikael Levi[1]; Jun Watanabe[1]; [1]*Shimadzu corporation, Kyoto, Japan*

ThP 083   **Detection of hormones (E1, E2, EE2) according to the requirements of the EU Water Framework Directive using an online-SPE-HPLC-MS/MS**; Fabian Itzel[1, 2]; Jill Kerstein[1]; Thorsten Teutenberg[1]; Jan Stenzler[3]; Stephane Moreau[4]; Jochen Tuerk[1, 2]; [1]*Institut für Energie- und Umwelttechnik e.V. – IUTA (Institut of Energy and Environmental Technology),, Duisburg, Germany; [2]Centre for Water and Environmental Research (ZWU), University of Duiburg-Essen, Duisburg, Germany; [3]Shimadzu Deutschland GmbH, Duisburg, Germany; [4]Shimadzu Europa GmbH, Duisburg, Germany*

ThP 084   **Fast determination of anionic polar pesticides and disinfection byproducts in homogenized food samples using ion chromatography and electrospray-ionization-mass spectrometry (IC-ESI-MS)**; Terri Christison[1]; Jeffrey S Rohrer[2]; [1]*Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 085   **Analysis of Glyphosate and Related Compounds in Drinking Water by Online SPE-UHPLC-MS/MS: A Method Development Story**; Jamie Foss[1]; Marjon Kuiper[2]; Boris Bartolec[2]; Peter Ringeling[2]; [1]*PerkinElmer, Shelton, CT; [2]Spark Holland B.V., Emmen, Netherlands*

ThP 086   **New biomarkers of exposure to the antidepressant venlafaxine in fish using suspect and non-target screening liquid chromatography-high resolution mass spectrometry**; Lucia H.M.L.M. Santos[1, 2]; Ana Luisa Maulvault[3]; Adrian Jaen-Gil[1, 2]; Antonio Marques[3]; Sara Rodriguez Mozaz[1, 2]; Damia Barcelo[1, 2, 4]; [1]*Catalan Institute for Water Research (ICRA), Girona, Spain; [2]University of Girona, Girona, Spain; [3]Portuguese Institute for the Sea and Atmosphere (IPMA, I.P.), Lisbon, Portugal; [4]IDAEA-CSIC, Barcelona, Spain*

ThP 087   **On-Demand Screening of Agrochemicals and Priority Pollutants in Soil Using Filter Cone Spray Ionization – Mass Spectrometry (FCSI-MS)**; Makoy R Overfelt[1]; Shahnaz Mukta[1]; Alyssa Gasa[1]; Christopher Mulligan[1]; [1]*Illinois State University, Normal, IL*

ThP 088   **A Validated UHPLC-MS/MS Method for the Identification of Aliskiren Photodegradation Products in Water**; Masho Hilawie Belay[1]; Fabio Gosetti[2]; Emilio Marengo[1]; Edoardo Pisano[1]; Jessica Luisetti[1]; Elisa Robotti[1]; [1]*Department of Science and Technological Innovations, University of Piemonte Orientale, Viale T. Michel 11, 15121 Alessandria, Italy; [2]Department of Earth and Environmental Sciences, University of Milano-Bicocca, Piazza della Scienza 1, 20126 Milano, Italy*

ThP 090   **Measurement of Underivatized Glyphosate and Other Polar Pesticides in Multiple Matrices Using Reversed-Phase Chromatography and Tandem Mass Spectrometry**; Jean-Francois Roy[1]; Jarod Grossman[2]; Sami Chanaa[3]; Tarun Anumol[3]; [1]*Agilent Technologies, Montreal, QC; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Wilmington, DE*

ThP 091   **Polar anticancer drugs in hospital and municipal wastewater by on-line extraction coupled to hydrophilic interaction liquid chromatography tandem mass spectrometry**; Marc-Antoine Vaudreuil[1]; Sung Vo Duy[1]; Gabriel Munoz[1]; Alexandra Furtos[1]; Sébastien Sauvé[1]; [1]*Université de Montréal, Montreal, QC*

ThP 092   **Determination of 33 pesticide residues in Lycium chinenseMill by GC-MS/MS**; Xiaodan Yang[1]; Chenyuan Zhang[1]; Jian Kang[1]; [1]*Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China*

ThP 093   **Analysis of Persistent Organic Pollutants in Drinking Water with Semi-Automated Solid Phase Extraction**; Tom Hall[1]; Ruud Addink[1]; [1]*Fluid Management Systems, Watertown, MA*

ThP 094   **Removal of 14 HIV/AIDS related drugs and 15 frequently detected pharmaceuticals using Moringa protein/PVA nanofibers andAnaphe pandafibers**; Temesgen Girma Kebede[1]; Simiso Dube-Nindi[1]; Mathew M Nindi[2]; [1]*UNIVERSITY OF SOUTH AFRICA(UNISA), Florida Park, Roodepoort, South Africa; [2]UNISA, Florida Park, Roodepoort, South Africa*

ThP 095   **Elucidation of environmental fate of Maprotiline and Aliskiren drugs in natural waters: Identification of degradation products via HPLC-HRMS**; Nuno P. F. Gonçalves[1]; Masho Hilawie Belay[2]; Elisa Robotti[2]; Claudio Medana[1]; Alessandra Bianco Prevot[1]; Paola Calza[1]; [1]*University of Turin, Turin, Italy; [2]University of Piemonte Orientale, Alessandria, Italy*

ThP 096   **Photodegradation of contaminants of emerging concern enhanced by dissolved organic matter derived from Pamvotis Lake sediments**; Cristina Jimenez-Holgado[1]; Sakkas Vasilios[1]; Richard Claire[2]; [1]*University of*

Ioannina, Ioannina, Greece; [2]Laboratoire de Photochimie moléculaire et Macromoléculaire, Clermont-Ferrand, France

ThP 097   **Iodinated X-ray Contrast Media as a Source of Iodine for the Formation of Iodinated DBPs Upon Chlorination During Wastewater Treatment**; Caroline O. Granger[1]; Hannah K. Liberatore[2]; Mark Ferrey[3]; Susan D. Richardson[1]; [1]*University of South Carolina, Columbia, SC; [2]US Environmental Protection Agency,, Raleigh, NC; [3]Minnesota Pollution Control Agency, St. Paul, MN*

ThP 098   **Screening of transformation products and intermediates from the aerobic degradation of oxytetracycline by HPLC-MS**; Federico Ivanic[1]; Matias Butler[1]; Roberto Candal[1]; [1]*Instituto de Investigación e Ingeniería Ambiental (IIIA, UNSAM), Buenos Aires, Argentina*

FOOD SAFETY: GENERAL II
ThP 099-117

ThP 099   **Food monitoring feasibility study on cereal: non-targeted food contaminants detection method development and semi-quantification model application using LC/HRMS**; Tingting Wang[1]; Jaanus Liigand[2]; Anneli Kruve[2, 3]; Lene Duedahl-Olesen[1]; [1]*National Food Institute, Technical University of Denmark, Lyngby, Denmark; [2]University of Tartu, Institute of Chemistry, Tartu, Estonia; [3]Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden*

ThP 100   **A simple dilute-and-shoot LCMS method for the determination of free and modified amino acids in dietary supplements**; Priyanka Chitranshi[1]; Jennifer C. Davis[1]; Evelyn H. Wang[1]; Christopher T. Gilles[1]; [1]*Shimadzu Scientific Instruments, Columbia, MD 21046*

ThP 101   **Electrospray Ionization Rapid Screening (ESI-RS) sans LC Column: Sensitive Method for the Determination of Chemicals in Animal Tissues and Urine**; Shubhashis Chakrabarty[1]; Weilin L Shelver[1]; David J Smith[1]; [1]*USDA, Fargo, ND*

ThP 102   **Development of simultaneous quantitative analysis of 18 anthelmintics in livestock products using liquid chromatography-tandem mass spectrometry**; Hae-Ni Jung[1]; Seong-Kwan Kim[1]; Da-Hee Park[1]; Kyung-Hee Yoo[1]; Ho-Chul Shin[1]; [1]*konkuk university, Seoul, South Korea*

ThP 103   **Multiresidue Pesticides Analysis in Food Matrices Using an Enhanced Triple Quadrupole LC/MS System**; Dan-Hui Dorothy Yang[1]; Kyle Covert[1]; Linfeng Wu[1]; [1]*Agilent Technologies, Santa Clara, CA*

ThP 104   **Direct Analysis of Glyphosate, Glufosinate and AMPA in Foods Using a Triple Quadrupole LC/MS/MS**; Miho Kawashima[1]; Kota Ishioka[2]; Manami Kobayashi[2]; Junichi Masuda[2]; Yoshihiro Hayakawa[1]; [1]*Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Corporation, Hadano, Japan*

ThP 105   **Comprehensive quantitative and qualitative analysis of aflatoxins by UHPLC coupled to a quadrupole-Orbitrap MS**; Laura E. Burns[1]; Dwayne E. Schrunk[1]; Viet Dang[2]; Dipankar Ghosh[2]; [1]*Iowa State Univ College of Veterinary Medicine, Ames, IA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 106   **Veterinary Drugs Screening in Food Tissues Using LDTD-MS/MS Technology**; Sylvain Letarte[1]; Pascal Belisle[1]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; [1]*Phytronix Technologies, Quebec, QC*

ThP 108   **A multiresidue pesticide method using a modified quadrupole-Orbitrap MS for quantitation, screening and confirmation**; Francesca Barbetti[1]; Charles T. Yang[2]; Debora D'adonna[3]; Christian Klass[4]; Dipankar Ghosh[2]; [1]*ISVEA S.r.L., Siena, Italy; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Milano, Italy; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 109   **Are there PFAS in my water? A detailed look into bottled water**; Brahm Prakash[1]; Eberhardt R Kuhn[1]; Ruth Marfil-Vega[1]; [1]*Shimadzu Scientific Instruments, Columbia, MD 21046*

ThP 110   **Separation of Mycotoxins by UHPLC-MS/MS using a Novel C18-based Stationary Phase**; Geoff Faden; *MAC-MOD Analytical, Chadds Ford, PA*

ThP 111   **LC-MS/MS Analysis of Glyphosate and Other Polar Contaminants in Food with a Novel Ion Exchange/HILIC Column**; Xiaoning Lu[1]; Dan Li[1]; Connor Flannery[1]; [1]*Restek Corporation, Bellefonte, PA*

ThP 112   **Protein Characterization by MALDI In-Source Decay Mass Spectrometry in Support of Safety Assessments of Genetically Modified Crops**; Ivan Birukou[1]; Scott Young[1]; Gerson Graser[1]; [1]*Syngenta Crop Protection, LLC, Research Triangle Park, NC*

ThP 113   **Dispersive Liquid-Liquid Microextraction of Chloramphenicol and its Congeners Residues in Water, Meat and Milk -ESI-LCMS/MS**; Ompelege E Kemokgatla[1]; Simiso Dube-Nindi[2]; Mathew M Nindi[3]; [1]*Residue Section, Botswana Nationa IVeterinary Laboratory,, Gaborone, Botswana; [2]UNIVERSITY OF SOUTH AFRICA(UNISA), Florida Park, Roodepoort, South Africa; [3]UNISA, Florida Park, Roodepoort, South Africa*

ThP 114   **Determination of mixed contaminants (mycotoxins, pesticides & veterinary) in food by green microextraction -Orbitrap HRMS**; Balete Esethu Gebreyohannes[1]; Simiso Dube-Nindi[1]; Mathew M Nindi[2];

[1]UNIVERSITY OF SOUTH AFRICA(UNISA), Florida Park, Roodepoort, South Africa; [2]UNISA, Florida Park, Roodepoort, South Africa

ThP 116 **Heavy Metals in Pet Food: Changes in Heavy Metal Contamination in Pet Food over the past Decade**; Patricia Atkins[1]; Tina Restivo[2]; Robert Lockerman[2]; *[1]SPEX CertiPrep, Metuchen, NJ; [2]CEM Corporation, Matthews, NC*

ThP 117 **Improving reproducibility and recovery by reducing ionization suppression of LC-MS/MS for quantitation of pesticide residues in chickpea powder**; Prasanth Joseph[1]; Parul Thakur[2]; Saikat Banerjee[1]; Samir Vyas[2]; *[1]Agilent Technologies, BENGALURU, India; [2]Agilent Technologies, Mumbai, India*

FORENSICS II
ThP 118-126

ThP 118 **Investigation of fires by unconventional IID (Improvised Incendiary Device) and combustion residues on different materials by SPME-GC-MS**; Marco Pazzi[1]; Sofia Ubaldi[1]; Eugenio Alladio[1, 2]; Fabrizio Malaspina[3]; Marco Vincenti[1, 2]; *[1]Dipartimento di Chimica, Universita' degli Studi di Torino, Torino, Italy; [2]Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole 10/1, 10043 Orbassano (Torino), Italy; [3]Corpo Nazionale dei Vigili del Fuoco – Comando di Torino, Unità d'intervento Nucleare Biologico Chimico Radiologico, Torino, Italy*

ThP 119 **An Ambient Mass Spectral Technique for the Rapid Detection of Cannabinoids in Plant Material and Complex Edible Matrices**; Megan I Chambers[1]; Rabi A Musah[1]; *[1]University at Albany - SUNY, Albany, NY*

ThP 120 **Identification of Compounds in the Environment of Equine Racing Facilities by LC-MS/MS**; Rachel Proctor[1, 2]; Youwen You[1, 2]; Jaclyn R Missanelli[1, 2]; Dominic M Giandonato[1, 2]; Joanne Haughan[1]; Mary A Robinson[1, 2]; *[1]University of Pennsylvania, Kennett Square, PA; [2]PA Equine Toxicology and Research Laboratory, West Chester, PA*

ThP 121 **Looking a decade back: hair testing for tracking history of self-reported opium use**; Elena V Romanova[1, 2]; Arash Etemadi[3, 4]; Reza Malekzadeh[5]; Jonathan D. Pollock[4, 6]; Jonathan V Sweedler[1, 2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]Beckman Institute, UIUC, Urbana, IL; [3]National Cancer Institute, Bethesda, MD; [4]NIH, Bethesda, Maryland; [5]Tehran University of Medical Sciences, Tehran, Iran; [6]National Institute on Drug Abuse, Bethesda, MD 20892*

ThP 122 **Direct Detection and Semi-Quantification of Illicit Drugs with the MasSpec Pen Coupled to Sub-Atmospheric Pressure Chemical Ionization**; Abigail N Gatmaitan[1]; Clara L Feider[1]; Jialing Zhang[1]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 123 **Screening and Analysis of 205 Illegal Drugs by High Resolution Mass Spectrometry**; Xiangjun Li; *ThermoFisher, Shanghai, China*

ThP 124 **Targeted and untargeted screening procedures in forensic toxicology. Evaluation of different instrumental technologies and analytical strategies**; Monica Mazzarino[1]; Fabio Comunità[1]; Xavier De La Torre[1]; Carlotta Stacchini[1]; Francesco Botrè[1]; *[1]Laboratorio Antidoping di Roma-Federazione Medico Sportiva Italiana, Rome, Italy*

ThP 125 **Drug Screening in Whole Blood Using a High-Resolution LC/Q-TOF and Novel Software Screener Tool**; Karen Yannell[1]; Manuel Gomez[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 126 **Identification and Confirmation of Fentanyls from Paper using Portable Surface Enhanced Raman and Paper Spray Ionization Mass Spectrometers**; Nicolas M Morato[1]; Patrick W. Fedick[1, 2]; Fan Pu[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Research Department, Chemistry Division, United States Navy - Naval Air Systems Command (NAVAIR), Naval Air Warfare Center, Weapons Division (NAWCWD), China Lake, CA*

FUNDAMENTALS: ION ACTIVATION/DISSOCIATION
ThP 127-138

ThP 127 **Unveiling the Hidden Complexity of Lithiated Hexose Dissociation Chemistry**; Paul S. Soma[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 128 **Comparison of ECD and UVPD for the relative quantitation of the isomeric products of deamidation**; Anisha Haris[1]; Yuko Lam[1]; Alina Theisen[1]; Christopher A. Wootton[1]; Tomos E. Morgan[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom*

ThP 129 **ESI mass spectral studies on L-arginine and model peptides containing arginines that are chemically modified by diketopinic acid**; Boomathi Pandeswari Pandi[1]; Varatharajan Sabareesh[1]; *[1]Advanced Centre for Bio Separation Technology (CBST), Vellore Institute of Technology (VIT), Vellore, India*

ThP 130 **Negative Ion In-Source Decay MALDI/TOF MS on Model Peptides**; Can Cui[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

ThP 131 **Formation and fragmentation of lithium acetate cluster ions studied by ESI-Orbitrap MS & HCD MS/MS and molecular dynamics simulations**; Bogdan Bogdanov[1]; Jincheng Zhang[2]; Andrew Parkins[3]; Anil K Shukla[4]; Michael Mccallum[3]; [1]*Shimadzu Scientific Instruments, Pleasanton, CA; [2]Beijing Normal University, Beijing, China; [3]Department of Chemistry, University of the Pacific, Stockton, CA; [4]Retired, Richland, WA*

ThP 132 **Improved Electron Capture Dissociation Tandem Mass Spectrometry of Post-translationally Modified Peptides via Collision Induced Unfolding**; Nhat Le[1]; Ruwan T. Kurulugama[2]; Varun V. Gadkari[1]; Chae Kyung Jeon[1]; Brandon Ruotolo[1]; Kristina Hakansson[1]; [1]*University of Michigan, Ann Arbor, Michigan; [2]Agilent Technologies, Santa Clara, CA*

ThP 133 **Screening of a Basic Side Chain on Acetylated and Nonacetylated Peptoids**; Yadwinder Singh Mann[1]; Yuntao Zhang[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

ThP 134 **Derivatization strategies for radical-directed dissociation: A radical renaissance for structure elucidation of small molecules in liquid chromatography-mass spectrometry**; Venkateswara R Narreddula[1]; Benjamin I Mckinnon[2]; Nathan RB Boase[1]; Berwyck LJ Poad[1]; David L Marshall[1]; Adam J Trevitt[2]; Todd W Mitchell[2]; Stephen J Blanksby[3]; [1]*Queensland University of Technology, Brisbane, Australia; [2]University of Wollongong, Wollongong, Australia; [3]Queensland University of Technology, Brisbane, Australia*

ThP 135 **Charge-remote Fragmentations of 3-Pyridinylboronic Esters of Saccharides in situ Formed in ESI by Triple Quadrupole Mass Spectrometry**; Jun J Hu[1]; Lei Li[1]; Pengfei Guan[1]; Pingping Wang[1]; [1]*Ningbo University, Ningbo, China*

ThP 136 **Variation of the Fragmentation Harshness of the Resonant Excitation Process in Quadrupole Ion Traps and Its Pressure Dependence**; Thomas Sebastian Neugebauer[1]; Antony Memboeuf[1]; [1]*CEMCA, Université de Brest, CNRS, Université Bretagne Loire, Brest, France*

ThP 137 **Fragmentation Behavior and Stability of Sulfated Peptides in Positive Ion Mode**; Eunju Jang[1]; Y-Linh Tran[1]; Kristina Hakansson[1]; [1]*University of Michigan, Ann Arbor, Michigan*

ThP 138 **Dynamics of the Collision-Induced Dissociation Process in Quadrupole Ion Traps**; Thomas Sebastian Neugebauer[1]; Thomas Drewello[2]; [1]*CEMCA, Université de Brest, CNRS, Université Bretagne Loire, Brest, France, Brest, France; [2]Friedrich-Alexander-University Erlangen-Nuremberg (FAU), Erlangen, Germany*

FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
ThP 139-151

ThP 139 **Formation of Carbon Dioxide Adducts from Carboxamide Anions Generated During Gas-Phase Fragmentation of Anions Derived from Capsaicinoids**; Annie Guan Wang[1]; Zhaoyu Zheng[1]; Athula B. Attygalle[1]; [1]*Stevens Institute of Technology, Hoboken, NJ*

ThP 140 **High-Throughput Mass Spectrometry Platform for Gas-Phase Reaction Screening under Ambient Conditions**; Dmytro S Kulyk[1]; Abraham Badu-Tawiah[1]; [1]*OSU, Columbus, OH*

ThP 141 **Vibrational excitation prior to electron-based fragmentation enhances formation of w-ions from doubly charged peptides**; Yury V. Vasil'ev[1, 2]; Michael C Hare[1]; Joe Beckman[1, 2]; [1]*e-MSion, Inc., Corvallis, OR; [2]Oregon State University, Corvallis, OR*

ThP 143 **Fragmentation and gas-phase reactions of diphenhydramine and analogues using AuNPs for Laser Desorption Ionization Mass Spectrometry**; Claire Eberle[1]; Katherine A. Stumpo[1]; [1]*University of Scranton, Scranton, PA*

ThP 144 **Structural elucidation of sodium- and potassium-cationized phosphatidylcholines using electron induced dissociation**; Tingting Yan[1]; Matthias-Erich Born[1]; Boone M. Prentice[1]; [1]*The University of Florida, Gainesville, FL*

ThP 145 **In-ESI HDX of carbohydrate-metal adducts in solvated ESI droplets: Effects of metal ions and counter ions**; O. Tara Liyanage[1]; Emvia I. Calixte[1]; Ana V. Quintero[1]; Jacob B. Hatvany[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

ThP 146 **Selective gas-phase Schiff base formation of phosphatidylserine lipids in imaging mass spectrometry using charge inversion ion/ion reactions**; Xizheng (colin) Diao[1]; Boone M. Prentice[1]; [1]*University of Florida Department of Chemistry, Gainesville, FL*

ThP 147 **Investigating the Solution Phase Chemistry of Cisplatin and Several Analogues by Electrospray Q-ToF High Resolution Mass Spectrometry**; Jason D Herrera[1]; Stephan B.H. Bach[1]; [1]*University of Texas at San Antonio, San Antonio, TX*

ThP 148 **Dissociation of negatively charged peptides by a strong electron beam: Electron Detachment Dissociation and negative ion Electron Capture Dissociation**; Irfan Younus[1]; Takashi Baba[1]; [1]*SCIEX, Concord, ON*

ThP 149 **Distonic radical pathways of N-containing aromatics + acetylene lead to PANHs: pre-reactive complexes are the kinetic gatekeepers**; Patrick Kelly[1]; Oisin Shiels[1]; Cameron Bright[1]; Stephen J. Blanksby[2]; Gabriel Da

Silva[3]; Adam Trevitt[1]; [1]*University of Wollongong, Wollongong, Australia;* [2]*Queensland University of Technology, Brisbane, Australia;* [3]*University of Melbourne, Parkville, Australia*

ThP 150 **Development of Negative Macromolecular Analyte Mass Analysis via Massive Ion Attachment (MAMA-MIA)**; Anthony M. Pitts-McCoy[1]; Abdirahman M. Abdillahi[1]; Kenneth W. Lee[1]; Scott A. Mcluckey[1]; [1]*Purdue University, West Lafayette, IN*

ThP 151 **Rate effects of submerged entrance barrier energetics on phenyl-type distonic radical ion reactions with acetylene**; Paddy Kelly[1]; Oisin Shiels[1]; Cameron Bright[1]; Brett Burns[1]; Jack Turner[1]; Gabriel Da Silva[2]; Stephen J. Blanksby[3]; Adam Trevitt[1]; [1]*University of Wollongong, Wollongong, Australia;* [2]*University of Melbourne, Parkville, Australia;* [3]*Queensland University of Technology, Brisbane, Australia*

FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS, CATALYSIS
ThP 152-157

ThP 152 **Molecular mechanism of ISC iron–sulfur cluster biogenesis revealed by high-resolution native mass spectrometry**; Cheng-Wei Lin[1]; Jacob W. McCabe[1]; David H. Russell[1]; David P. Barondeau[1]; [1]*Texas A&M University, College Station, TX*

ThP 153 **Simultaneous analysis of metal ions and organic components by HPLC-ESI-MS system**; Kuck-Fai Li[1]; Pai-Chi Syue[1]; Ching-Yi Lien[1]; Kuo-Lung Ku[1]; [1]*National Chiayi University, Chiayi City, Taiwan*

ThP 154 **Real-time stepwise analysis of palladium catalysis**; Gilian Thomas[1]; Scott Mcindoe[2]; [1]*University of Victoria, Victoria, BC;* [2]*University of Victoria, Victoria, British Columbia*

ThP 155 **Lithium Cation Basicity Estimates of Lignin β-0-4 Dimers**; Kimberly R Dean[1]; Bert C. Lynn[1]; [1]*University of Kentucky, Lexington, KY*

ThP 156 **Hydrocarbon Formation Through Decomposition of Fatty Acids Catalyzed by Metal Complexes in the Gas Phase**; Kevin E Parker[1]; Geethi Weragoda[2]; Richard O'hair[3]; Victor Ryzhov[1]; [1]*Northern Illinois University, DeKalb, IL;* [2]*CSIRO Manufacturing, Clayton, Australia;* [3]*School of Chemistry, University of Melbourne, Parkville, Australia*

ThP 157 **Dissociation of mass-isolated encounter complexes of platinum(IV) prodrugs and ascorbic acid elucidates details on their bioactivation**; Davide Corinti[1]; Maria Elisa Crestoni[1]; Simonetta Fornarini[1]; Eslam Dabbish[2]; Emilia Sicilia[2]; Elisabetta Gabano[3]; Elena Perin[3]; Domenico Osella[3]; [1]*Università di Roma "La Sapienza", Roma, Italy;* [2]*Università della Calabria, Arcavacata di Rende, Italy;* [3]*Università del Piemonte Orientale, Alessandria, Italy*

FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS
ThP 158-161

ThP 158 **Comparison of Fragmentation of Zn(II)-2Cys-2His Model Oligopeptide using Direct Dynamics Simulations and Mass Spectrometry**; Abdul Malik[1]; William L. Hase[2]; Laurence A Angel[3]; [1]*Texas Tech University, Lubbock, TX;* [2]*Texas Tech University - Lubbock, TX, Lubbock, TX;* [3]*Texas A&M University, College Station, TX*

ThP 159 **Theoretical Calculation of Nonpolar Surface Areas with Implicit Solvent Methods and Its Application in Glycomics/Glycoproteomics Analysis**; Daniel De Castro Araujo Valente[1]; Rabin Dhakal[2]; Wenjing Peng[2]; Reed Nieman[2]; Adelia J. A. Aquino[2]; Hans Lischka[2]; Yehia Mechref[2]; [1]*Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil;* [2]*Texas Tech University, Lubbock, TX*

ThP 160 **An Application of DFT for Characterizing the Energetics of HDX for Solvated Glucose**; Meg Mccutcheon[1]; Emvia Calixte[1]; Emily Ziperman[1]; H. Jamie Kim[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

ThP 161 **Comparing Collisional Cross Sections of N-Acetyl Modified Carbohydrates to Determine Computational Model Accuracy and Precision**; Emily D Ziperman[1]; Emvia I Calixte[1]; Meg E McCutcheon[1]; Srinivas Pulipaka[1]; Elyssia S Gallagher[1]; [1]*Baylor University, Waco, TX*

FUNDAMENTALS: NATIVE MS
ThP 162-170

ThP 162 **Implementation of surface-induced dissociation on an Orbitrap EMR via the HCD cell using a reverse-entry ion source**; Benjamin J Jones[1, 2]; Jacob W. McCabe[2, 3]; Dalton T. Snyder[1, 2]; Zachary L VanAernum[1, 2]; Sophie R. Harvey[1, 2]; David H. Russell[2, 3]; Vicki H. Wysocki[1, 2]; [1]*The Ohio State University, Columbus, OH;* [2]*Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH;* [3]*Texas A&M, College Station, TX*

ThP 163 **Switch of dissociation channels in native top-down MS of protein complexes and its implications for topology analysis**; Guanbo Wang[1]; Albert J. R. Heck[2]; Wenjun Tong[1]; Jianbin Wang[3]; [1]*Nanjing Normal University, Nanjing, China;* [2]*Utrecht University, Utrecht, Netherlands;* [3]*Tsinghua University, Beijing, China*

ThP 164 **Surface-induced dissociation of protein complexes on a cyclic ion mobility spectrometer**; Dalton T Snyder[1]; Ben Jones[1]; Leon Lin[1]; Alyssa Stiving[1]; Sophie Harvey[1]; Vicki H Wysocki[1]; Darren Hewitt[2]; Jason Wildgoose[2]; Dale A. Cooper-Shepherd[2]; Jeffrey M. Brown[2]; Jakub Ujma[2]; Jim Langridge[2]; [1]*The Ohio State University, Columbus, OH;* [2]*Waters Technologies, Wilmslow, United Kingdom*

ThP 165 **Molecular weight determination of an adeno-associated virus based virus-like particle**; Samuele Zoratto[1]; Victor U. Weiss[1]; Martina Marchetti-Deschmann[1]; Elisabeth Mueller[2]; Robert Pletzenauer[2]; Juan Hernandez Bort[2]; Guenter Allmaier[1]; [1]*TU Wien, Vienna, Austria;* [2]*Takeda Austria GmbH, Vienna, Austria*

ThP 166 **Native ESI MS for Deep Characterization of JMJD3 and JMJD3-Binder Interactions**; Xidong Feng[1]; Yue Feng[2]; Timothy Foley[1]; Dafydd Owen[3]; [1]*Pfizer, Groton, CT;* [2]*Spectrix Analytical Services, North Haven, CT 06473;* [3]*Pfizer, Cambridge, MA*

ThP 167 **Probing the gas-phase structure of lipoprotein nanodiscs using surface-induced dissociation**; Sophie R Harvey[1]; Zachary L Vanaernum[1]; Marius M Kostelic[2]; Michael T Marty[2]; Vicki H Wysocki[1]; [1]*The Ohio State University, Columbus, OH;* [2]*University of Arizona, Tucson, AZ*

ThP 168 **A Microflow LC-MS Platform for Native Protein Analysis**; Weimin Ni[1]; Maoyin Li[1]; Yan Han[1]; Pan Mao[1]; Daojing Wang[1]; [1]*Newomics Inc., Berkeley, CA*

ThP 169 **Screening tagged proteins using online tandem affinity-buffer exchange chromatography with native mass spectrometry**; Stella M. Lai[1, 2]; Zachary L. VanAernum[1, 2]; Florian Busch[1, 2, 3]; Julia Baek[4]; Terry Zhang[5]; Kyle L. Fort[6]; Rosa Viner[5]; Vicki H. Wysocki[1, 2, 3]; [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;* [3]*Campus Chemical Instrument Center, Mass Spectrometry and Proteomics, The Ohio State University, Columbus, OH;* [4]*Thermo Fisher Scientific, Sunnyvale, CA;* [5]*Thermo Fisher Scientific, San Jose, CA;* [6]*Thermo Fisher Scientific, Bremen, Germany*

ThP 170 **So HowBad is Ammonium Acetate for Native Mass Spectrometry? pH Changes During Nanoelectrospray Ionization (nESI) Quantified Using Fluorescence Imaging**; Matthew F. Bush[1]; Evan E Hubbard[2]; Meagan Gadzuk-Shea[1]; [1]*University of Washington, Seattle, WA;* [2]*University of California, Riverside, Riverside, CA*

GC/MS: INSTRUMENTATION AND APPLICATIONS
ThP 171-192

ThP 171 **Determination of 33 pesticide residues in Ginseng using gas chromatography-triple quadrupole mass spectrometry**; Xiaoming Bao[1]; Yan Gou[2]; Jun Fan[3]; Taohong Huang[3]; [1]*Shimadzu (China) Co., Ltd, Chengdu, China;* [2]*Sichuan Institute for Food and Drug Control, Chengdu, China;* [3]*Shimadzu (China) Co., Ltd, Shanghai, China*

ThP 172 **Thermal Desorption-GCMS Method for Screening of Extractables in in Drug Packaging Materials**; Cynthia Melanie Lahey[1]; Elgin Guo Wei Ting[1]; Dheeraj Handique[2]; Yukihiko Kudo[3]; [1]*Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore;* [2]*Shimadzu Analytical (India) Pvt Ltd, Mumbai, India;* [3]*Shimadzu Corporation, Kyoto, Japan*

ThP 173 **Determination of PAEs in marine environment by GCMS**; Gang Huang; *shimadzu, GuanZhou, China*

ThP 174 **VOC Capturing Method for Odor Smell Analysis by GC-MS**; Takeshi Furuhashi[1]; Shigenori Ota[2]; [1]*Anicom Specialty Medicinal Institute, Yokohama, Japan;* [2]*GL Sciences Inc., Shinjuku-Ku, Japan*

ThP 175 **Medical Diagnostics by GC-MS with Cold EI – Lipids and Drugs Analysis in Raw Blood**; Benjamin Neumark[1]; Aviv Amirav[1, 2]; [1]*Tel Aviv University, Tel Aviv, Israel;* [2]*Aviv Analytical, Hod Hasharon, Israel*

ThP 176 **Integrated qualitative analysis of polymer samples by a pyrolysis - gas chromatography combined with high-resolution mass spectrometry**; Masaaki Ubukata[1]; Ayumi Kubo[1]; Kenji Nagatomo[1]; Robert A. Dipasquale[2]; [1]*JEOL, Ltd., Tokyo, Japan;* [2]*JEOL USA, Inc., Peabody, MA*

ThP 177 **Optimum molecular descriptors based on 89 machine learning methods for predicting the recovery rate of pesticides in crops by GC-MS**; Takeshi Serino[1, 2]; Yoshizumi Takigawa[1]; Sadao Nakamura[1]; Tarun Anumol[3]; Md. Altaf-UI-Amin[2]; Shigehiko Kanaya[2]; [1]*Agilent Technologies, Hachioji, Japan;* [2]*Nara Institute of Science and Technology, Ikoma, Japan;* [3]*Agilent Technologies, Wilmington, DE*

ThP 178 **IDENTIFYING BEST APPROACHES TO ANALYZE VOLATILE EXTRACTABLES FROM MEDICAL DEVICES**; Samanthi I Wickramasekara[1]; Keaton Nahan[1]; Eric Sussman[1]; Berk Oktem[1]; [1]*US.Food and Drug Administration, Silver Spring, MD*

ThP 179 **Determination of Dioxin in Food by GCMSMS coupled with Boosted Efficiency Ion Source (BEIS)**; Ge Yin[1]; Feifei Tian[2]; Jun Fan[1]; Masato Takakura[3]; Koki Tanaka[3]; Eberhardt Kuhn[4]; Dan Luo[5]; Taohong Huang[1]; [1]*Shimadzu China, Shanghai, China;* [2]*Shimadzu, Beijing, China;* [3]*Shimadzu Corpration, Kyoto, Japan;* [4]*Shimadzu Scientific Instruments, Inc, Columbia, MD;* [5]*Shimadzu China, Wuhan, China*

ThP 180 **Quantitative Multiplexed Elemental (C, H, N and S) Detection in Complex Mixtures using Gas Chromatography-combustion-mass spectrometry**; Laura Freije-Carrelo[1]; Javier García-Bellido[1]; Laura Alonso Sobrado[1]; Mariella Moldovan[1]; Marco Piparo[2, 3]; Brice Bouyssiere[3, 4]; Pierre Giusti[2, 3]; Jorge Ruiz-Encinar[1]; [1]*Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, Spain;* [2]*TOTAL, Harfleur, France;* [3]*International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France;* [4]*Universite de Pau et des Pays de l'Adour, E2S UPPA, CNRS, IPREM, UMR5254, Pau, France*

ThP 181 **A Multi Mode Ion Source for GCxGC-HR-TOFMS Applications**; George Tikhonov[1]; Scott Pugh[1]; Viatcheslav Artaev[1]; [1]*LECO Corporation, Saint Joseph, MI*

ThP 182 **Derivatization and Quantitation of Formaldehyde using PFBHA and Vacuum-Assisted Sorbent Extraction (VASE)**; Mitham Al-faliti[1]; Ashraf Hassan[2]; Sage Dunham[3]; Victoria L. Noad[3]; Daniel B. Cardin[3]; [1]*University of Nebraska - Lincoln, Lincoln, NE;* [2]*University of Nebraska-Lincoln, Lincoln, NE;* [3]*Entech Instruments Inc, Simi Valley, CA*

ThP 183 **Simultaneous analysis of NDMA, NDEA, NDIPA and NEIPA impurities in valsartan drug substance and drug products using Headspace GC/MS**; Diaa Shakleya[1]; Susan (daniela) Selaya[1]; Patrick Faustino[1]; [1]*FDA, Silver Spring, MD*

ThP 184 **Black Pepper authenticity workflow using high-resolution GC/Q-TOF**; Sofia Nieto[1]; Melissa Churley[1]; [1]*Agilent Technologies, Inc., Santa Clara, CA*

ThP 185 **On-line Automated Derivatization of Free Fatty Acids for High-Throughput Fatty Acid Profiling**; Paul J Gries[1]; Stefano Tiziani[1]; [1]*The University of Texas at Austin, Austin, TX*

ThP 186 **Qualitative and quantitative assessment of flavor from cucumis melo using gas chromatography electron and chemical ionization mass spectrometry**; Rita V Metrani[1, 2]; Jashbir Singh[1, 2]; G. K. Jayaprakasha[1, 2]; Bhimanagouda S. Patil[1, 2]; [1]*Vegetable and Fruit Improvement Center, College Station, TX;* [2]*Texas A&M University, College Station, TX*

ThP 187 **Rinse and Shoot: Pesticide Screening Workflow by GC/MS in Under Five Minutes**; Anastasia Andrianova[1]; Bruce Quimby[1]; [1]*Agilent Technologies, Wilmington, DE*

ThP 188 **Analysis of Semi-Volatile Organics in Drinking Water with Semi-Automated Solid Phase Extraction Using EPA Method 525.3**; Rudolf Addink[1]; Tom Hall[1]; [1]*Toxic Report, Watertown, MA*

ThP 189 **High Throughput Semi Automated Solid Phase Extraction and Analysis of Waste Water Using EPA 8270D**; Tom Hall[1]; Ruud Addink[1]; Garvey Mckenzie[1]; [1]*Fluid Management Systems, Watertown, MA*

ThP 190 **GCxGC-HRTOF-MS of Volatile Organic Signatures of Antimicrobial Resistance in Yersinia pestis and Francisella tularensis**; Brooke L. Deatherage Kaiser[1]; Jon Wahl[1]; Janine Hutchinson[1]; Sarah Jenson[1]; Cynthia Warner[1]; Alejandro Heredia-Langner[1]; David S Wunschel[1]; Dawn Birdsall[2]; David M Wagner[2]; Mats Forsman[3]; Johanna Thelaus[3]; Mona Bystrom[3]; Minoarisoa Rajerison[4]; Voahangy Andrianaivoarimana[4]; Richard A. Bowen[5]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Northern Arizona University, Flagstaff, AZ;* [3]*Swedish Defence Research Agency, Umea, Sweden;* [4]*Institute Pasteur Madagascar, Antananarivo, Madagascar;* [5]*Colorado State University, Fort Collins, CO*

ThP 191 **Implementation of Fisher ratio analysis for metabolite discovery in pacu fish using comprehensive two-dimensional gas chromatography with mass spectrometry**; Sonia Schöneich[1]; Sarah E. Prebihalo[1]; Celina Monzòn[2]; Robert E. Synovec[1]; [1]*University of Washington, Seattle, WA;* [2]*Universidad Nacional del Nordeste, Corrientes, Argentina*

ThP 192 **Implementation of Fisher ratio analysis to improve classification of sulfur-contaminated jet fuels using comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry data**; Paige E. Sudol[1]; Grant S. Ochoa[1]; Robert E. Synovec[1]; [1]*University of Washington, Seattle, WA*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION
ThP 193-210

ThP 193 **Perfluoroalkyl Substances (PFAS) Bind to Human Plasma Transthyretin (hTTR) in the Thyroxine-Binding Site: an HDX-MS Study**; Daniele Peterle[1]; Laura Acquasaliente[1]; Luca De Toni[2]; Carlo Foresta[2]; Barbara Spolaore[1]; Vincenzo De Filippis[1]; [1]*Department of Pharmaceutical and Pharmacological Sciences, Laboratory of Protein Chemistry and Molecular Haematology, University of Padua, Padua, Italy;* [2]*Department of Medicine, Unit of Andrology and Reproductive Medicine, School of Medicine, University of Padua, Padua, Italy*

ThP 194 **HDX-MS Reveals the assembly pathway of an encapsulated Ferritin**; Thomas Ole Tandrup Lambert[1]; Jennifer Ross[1]; Cecilia Piergentili[2]; Kevin Waldron[2]; Didi He[3]; Jon Marles-Wright[2]; Colin Logan Mackay[1]; David Clarke[1]; [1]*University of Edinburgh, Edinburgh, United Kingdom;* [2]*University of Newcastle, Newcastle, United Kingdom;* [3]*University of Oxford, Oxford, United Kingdom*

ThP 195 **Using Mass Spectrometry Based Structural Techniques to Study How Flavin-Dependent Oxidoreductase Converts Carbon Dioxide into Biomass**; Jenna Mattice[1]; Angela Patterson[1]; Bennett Streit[1]; John Peters[2]; Jennifer Dubois[1]; Brian Bothner[1]; [1]*Montana State University, Bozeman, MT;* [2]*Washington State University, Pullman, WA*

ThP 196 **Thermal activation networks in adenosine deaminase identified using hydrogen/deuterium exchange mass spectrometry**; Anthony T. Iavarone[1]; Shuaihua Gao[1]; Samuel L. Barrow[1]; Emily J. Thompson[1]; Wenju Zhang[2]; Judith P. Klinman[1]; [1]*University of California, Berkeley, Berkeley, CA;* [2]*University of Waterloo, Waterloo, ON*

ThP 198 **Investigating the relationship between hydrogen deuterium exchange and covalent labeling mass spectrometry in the context of antigen/antibody binding**; Catherine Tremblay[1]; Richard W Vachet[1]; Eric Graban[2]; John E. Hale[2]; Robert C. Vaughn[2, 3]; [1]*University of Massachusetts Amherst, Amherst, MA;* [2]*QuarryBio LLC, Bloomington, IL;* [3]*Indiana University, Bloomington, IN*

ThP 199 **Two Binding Modes, One Nuclear Receptor: Analyzing Chemopreventative Rexinoids using Hydrogen Deuterium Exchange Mass Spectrometry**; Nathalia Melo[1]; Zhengrong Yang[1]; Sejong Bae[1]; Venkatram Atigadda[1]; Donald D. Muccio[1]; Matthew Renfrow[1]; [1]*University of Alabama at Birmingham, Birmingham, AL*

ThP 200 **Conformational Dynamics of TEM-type Extended Spectrum β-Lactamases as Revealed by HDX-MS**; Tsz Fung Wong[1]; Pui Kin So[1]; Zhongping Yao[1]; [1]*The Hong Kong Polytechnic University, Hong Kong, Hong Kong*

ThP 201 **Mapping activation mechanisms in proline-rich tyrosine kinase 2 by H/D exchange mass spectrometry;** Hanna S Loving; Tania M Palhano Zanela; Eric Underbakke; *Iowa State University, Ames, IA, United States*

ThP 202 **HDX-MS for epitope characterization of an antibody drug candidate on the highly structured, calcium-binding protein Annexin A1**; Marius Gramlich[1]; Henry C.W. Hays[2]; Dieter Stoll[1, 3]; Sandra Maier[1]; Anne Zeck[1]; [1]*Natural and Medical Science Institute at the University of Tuebingen, Reutlingen, Germany;* [2]*MedAnnex, Edinburgh, United Kingdom;* [3]*University of Applied Sciences Albstadt-Sigmaringen, Sigmaringen, Germany*

ThP 203 **Detailed, protein-wide effects of crosslinking on the conformation and dynamics of native states revealed by HDX**; Frederik Lermyte[1, 2]; Emeline Hanozin[2]; Thomas Tilmant[2]; Johann Far[2]; Loïc Quinton[2]; Edwin De Pauw[2]; Gauthier Eppe[2]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*University of Liege, Liège, Belgium*

ThP 204 **Characterizing Small Molecule Inhibitors of CK2 Kinase Subunit α by HDX-MS**; Darby J Ball[1]; Paul Brear[2]; Marko Hyvönen[3]; Sheena D'arcy[4]; [1]*University of Texas at Dallas, Richardson, TX;* [2]*Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom;* [3]*2Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom;* [4]*Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas*

ThP 205 **Impact of Catalytic Site Residues Mutation on Structure, Conformational Gating and Dynamics of Human Monoacylglycerol Lipase**; Ioannis Karageorgos[1]; Sergiy Tyukhtenko[2]; Girija Rajarshi[2]; Kyle Anderson[1]; Jeffrey W Hudgens[1]; Mahmoud Nasr[3]; Nikolai Zvonok[2]; Jason Guo[2]; Kiran Vemuri[2]; Gerhard Wagner[3]; Alexandros Makriyannis[2]; [1]*NIST, Rockville, MD;* [2]*Northeastern University, Boston, MA;* [3]*Harvard Medical School, Boston, MA*

ThP 206 **HDX-MS guided modeling and ensemble reweighting approach to characterize the structure and dynamics of cytoplasmic heme binding protein PhuS**; Kyle Kihn[1]; Patrick L. Wintrode[1]; Daniel J. Deredge[1]; [1]*University of Maryland School of Pharmacy, Baltimore, MD*

ThP 207 **Refined Analysis of Calprotectin-Calcium Binding by Use of Three Titration MS Measurement Methods: HDEX, Sharp-break HDEX and Native Spray**; Jagat Adhikari[1]; Jules R. Stephan[2]; Don L Rempel[1]; Elizabeth M. Nolan[2]; Michael L. Gross[1]; [1]*Department of Chemistry, Washington University at St Louis, St. Louis, MO 63130;* [2]*Department of Chemistry, Massachusetts Institute of Technology, Boston, MA 02139*

ThP 208 **Mapping the interaction surface of two critical protein quality control mechanism players, BAG-1S and VCP/p97, using HDX-MS**; Ezgi Basturk[1]; Ozge Tatli[1, 2]; Gizem Dinler Doganay[1]; [1]*Istanbul Technical University, Istanbul, Turkey;* [2]*Istanbul Medeniyet University, Istanbul, Turkey*

ThP 209 **Mass Spectrometry Based Structural Analysis of the Zika NS1 Protein in the Presence or Absence of Several Zika Virus Antibodies**; Prashant N. Jethva[1]; Alex W. Wessel[2]; Christopher A. Nelson[3]; Nurgun Kose[4, 5, 6]; James E. Crowe, Jr. [4, 5, 6]; Michael S. Diamond[2, 3, 7]; Daved H. Fremont[3, 7, 8]; Michael L. Gross[1]; [1]*Department of Chemistry, Washington University in St. Louis, Saint Louis, MO-63130;* [2]*Department of Medicine, Washington University School of Medicine, Saint Louis, MO-63110;* [3]*Department of Pathology and Immunology, Washington University School of Medicine, Saint Louis, MO-63110;* [4]*Vanderbilt Vaccine Center, Vanderbilt University Medical Center, Nashville, TN-37232;* [5]*Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN-37232;* [6]*Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN-37232;* [7]*Department of Molecular Microbiology, Washington University School of Medicine, Saint Louis, MO-63110;* [8]*Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, Saint Louis, MO-63110*

ThP 210 **Dynamics and networking in secretory chaperones using Native and hydrogen-deuterium exchange Mass spectrometry**; Bindu Y Srinivasu[1]; Athina G Portaliou[1]; Anastassios Economou[1]; Spyridoula Karamanou[1]; [1]*KU Leuven, Leuven, Belgium*

HIGH MASS ACCURACY/HIGH PERFORMANCE MS: APPLICATIONS AND INSTRUMENTATION
ThP 211-219

ThP 211 **Towards Applying High Resolution Mass Spectrometry for Quantitative Source Apportionment: Evaluating Matrix Effects and Non-target Signature Fidelity**; Katherine T Peter[1]; Zhenyu Tian[2]; Christopher Wu[2]; Edward P Kolodziej[2, 3]; John Kucklick[1]; [1]*National Institute of Standards and Technology, Charleston, SC;* [2]*Center for Urban Waters, University of Washington Tacoma, Tacoma, WA;* [3]*University of Washington, Seattle, WA*

ThP 212   **Confident LC-MS identification of low ppm host cell proteins (HCP) in biotherapeutic monoclonal antibodies**; Amy J Claydon[1]; Philip J Widdowson[1]; Andrew Williamson[2]; Min Du[3]; [1]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [2]*Thermo Fisher Scientific, Hemel Hempstead, United Kingdom;* [3]*Thermo Fisher Scientific, Cambridge, MA*

ThP 213   **Is High-Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Needed to Improve Metabolite Annotation?**; Danning Huang[1]; Marcos Bouza Areces[1]; David A. Gaul[1]; Arthur S. Edison[2]; Facundo M. Fernandez[1]; [1]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia;* [2]*Department of Genetics and Biochemistry and Molecular Biology, Complex Carbohydrate Research Center, University of Georgia, Athens, Georgia*

ThP 214   **Comparison of Orbitrap Mass Accuracy Using External and Internal Lock Mass Correction Methods**; Christopher Mullen[1]; Jesse D Canterbury[1]; Graeme Mcalister[1]; Michael Goodwin[1]; Arne Kreutzmann[2]; Romain Huguet[1]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Bremen, Germany*

ThP 215   **Structural Determination at the Chemical Formula Level using TIMS-FT-ICR MS/MS**; Dennys Leyva[1]; Rudolf Jaffé[1]; Francisco A. Fernandez-Lima[1]; [1]*Florida International University, Miami, FL*

ThP 216   **Effect of postnatal alcohol exposure on protein synthesis in developing rat liver**; Sergei Ilchenko[1]; Ella Alvarado[1]; Mirjavid Ahgayev[1]; Andrew Haddad[1]; Takhar Kasumov[1]; Nadia Rachdaoui[2]; [1]*Northeast Ohio Medical University, Rootstown, OH;* [2]*Rutgers University, New Brunswick, NJ*

ThP 217   **Comprehensive study of protein aggregation with ultra-high resolution mass spectrometry and surface-induced dissociation**; Mehdi Shirzadeh[1]; Zahra Moghadamchargari[1]; Jacob W. McCabe[1]; Arthur Laganowsky[1]; David H. Russell[1]; [1]*Texas A&M University, College Station, TX*

ThP 218   **Rapid quantification of small molecules in biofluids by capillary vibrating sharp-edge spray ionization (cVSSI) and solid-phase microextraction (SPME) mass spectrometry**; Jing Wang[1]; Chong Li[1]; Stephen J Valentine[1]; Peng Li[1]; [1]*West Virginia University, Morgantown*

ThP 219   **Unambiguous di-sulphide bond assignment in synthetic therapeutic peptides Linaclotide and Plecanatide using Agilent 6546 LC-QTOF High Resolution Mass Spectrometer**; Srinivasulu Polisetty[1]; Laxmi Katta Reddy[1]; Venkat Reddy[1]; Ashish Pargaonkar[2]; Saikat Banerjee[3]; Saurabh Nagpal[4]; [1]*MSNL R&D Center Pashamylaram, Medak District, India;* [2]*Agilent Technologies, BENGALURU, India;* [3]*Agilent Technologies India Pvt Ltd, Hyderabad, India;* [4]*Agilent technologies, Gurgaon, India*

IMAGING MS: METHOD DEVELOPMENT
ThP 220-247

ThP 220   **A high efficient and wide coverage mass spectrometry imaging method for broad functional metabolite discovery in ischemic stroke model**; Zixuan Wang[1]; Ran Yang[1]; Xin Li[1]; Zeper Abliz[1, 2]; [1]*Institute of Materia, Chinese Academy of Medical Science and Peking Union Medical College, Beijing, China;* [2]*Minzu University of China, Beijing, China*

ThP 221   **Spatial Localization of Vitamin D metabolites in Mouse Kidney by Mass Spectrometry Imaging**; Karl Smith[1]; Bryn Flinders[2]; Paul Thompson[3]; Faye Cruickshank[4]; C. Logan Mackay[4]; Ron M.A Heeren[5]; Diego F Cobice[1]; [1]*Mass Spectrometry Centre, Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University, Coleraine, United Kingdom;* [2]*Dutch Screening Group, Maastricht, Netherlands;* [3]*The Nutrition Innovation Centre for Food and Health (NICHE), Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University, Coleraine, United Kingdom;* [4]*Scottish Instrumentation and Research Centre for Advanced Mass Spectrometry (SIRCAMS), EaStCHEM School of Chemistry, University of Edinburgh, Edinburgh, United Kingdom;* [5]*M4I institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands*

ThP 222   **Laser-induced post-ionization coupled to a timsTOF fleX for the enhanced MALDI-2-MS analysis of N-glycans**; Bram Heijs[1, 2]; Alexander Potthoff[1]; Hans Dalebout[2]; Jens Soltwisch[1, 3]; Klaus Dreisewerd[1, 3]; [1]*Institute of Hygiene, University of Muenster, Muenster, Germany;* [2]*Center for Proteomics and Metabolomics, Leiden, Netherlands;* [3]*Interdisciplinary Center for Clinical Research (IZKF), Muenster, Germany*

ThP 223   **MALDI Mass Spectrometry Imaging of Human Penile Tissue Scaffolds following Organ Decellularization to Evaluate Extracellular Matrix Preservation**; Caitlin Tressler[1]; Allister Suarez[1]; Yu Tan[1]; Wilmina Landford[1]; Devin Coon[1]; Kristine Glunde[1]; [1]*Johns Hopkins University School of Medicine, Baltimore, Maryland*

ThP 224   **Interlaboratory evaluation of MALDI and DESI MSI in the CRUK Grand Challenge programme**; Melina Kyriazi[1, 2]; Teresa Murta[2]; Chelsea Nikula[2]; Alex Dexter[2]; Adam Taylor[2]; Richard Goodwin[3]; Zoltan Takats[1]; Josephine Bunch[1, 2]; [1]*Imperial College London, London, United Kingdom;* [2]*National Physical Laboratory, Teddington, United Kingdom;* [3]*AstraZeneca, BioPharmaceuticals R&D, Imaging and AI, Clinical Pharmacology and Safety Sciences, Cambridge, United Kingdom*

ThP 225   **Versatile applications of MS imaging using a bench-top linear MALDI-TOFMS**; Yuzo Yamazaki[1]; Shuuichi Nakaya[2]; Catherine Rawlins[3]; Simona Salivo[3]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan;* [3]*Shimadzu, Manchester, UK, Manchester, United Kingdom*

ThP 226 **Progress in biopharmaceutical detection in an aggregated 3D cell culture model by multimodal mass spectrometry imaging**; Lucy E Flint[1]; Gregory Hamm[2]; Neil A Cross[1]; Laura M Cole[1]; David P Smith[1]; Richard Goodwin[2]; Malcolm R Clench[1]; [1]*Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom;* [2]*Pathology, Drug Safety & Metabolism, IMED Biotech Unit, AstraZeneca, Darwin Building, Cambridge Science Park, Cambridge, United Kingdom*

ThP 227 **Mass Spectrometry Imaging for the mapping of lipids using a DESI SYNAPT**; Ludovic Muller[1]; Ann M. Farese[2]; Thomas J. MacVittie[2]; Maureen A. Kane[1]; [1]*University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD;* [2]*University of Maryland, School of Medicine, Department of Radiation Oncology, Baltimore, MD*

ThP 228 **Method Development for using AuNPs in Mass Spectrometry Imaging**; Tyler M. Bielinski[1]; Nolan K Mclaughlin[1]; Caitlin M. Tressler[2]; Eric Barton[2]; Kristine Glunde[2]; Katherine A. Stumpo[1]; [1]*University of Scranton, Scranton, PA;* [2]*Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 229 **Imaging Mass Spectrometry of Insoluble Proteins**; Kevin L. Schey[1]; David M Anderson[2]; Zhen Wang[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Vanderbilt Unviersity, Nashville, TN*

ThP 230 **MALDI mass spectrometry imaging in aquatic model systems**; Elisabeth Schirmer[1, 2]; Axel Treu[1]; Sven Ritschar[3]; Stefan Schuster[2]; Christian Laforsch[3]; Andreas Römpp[1]; [1]*Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany;* [2]*Chair of Animal Physiology, University of Bayreuth, Bayreuth, Germany;* [3]*Chair of Animal Ecology I, University of Bayreuth, Bayreuth, Germany*

ThP 231 **Large scale MALDI-MS imaging of mammalian cell cultures at single cell resolution**; Jakob Meier-Credo[1]; Tejaswi Kalavacherla[1]; Erin M. Schuman[2]; Hartmut Michel[1]; Julian D. Langer[1, 2]; [1]*Max Planck Institute of Biophysics, Frankfurt, Germany;* [2]*Max Planck Institute for Brain Research, Frankfurt, Germany*

ThP 232 **Robotic Spotting for Quantitation and Mass Spectrometry Imaging by Combining MALDI and Laser Desorption Ionization from Silicon Nanopost Arrays**; Sara K Mattson[1]; Akos Vertes[1]; [1]*The George Washington University, Washington, DC*

ThP 233 **Mapping and identifying significant peptides in adult, female cattle fever ticks using mass spectrometry imaging and MALDI-TOF/TOF**; Grace Samenuk[1]; Stephan B.H. Bach[2]; Adalberto Pérez De León[3]; [1]*University of Texas at San Antonio, San Antonio, TX;* [2]*University of Texas in San Antonio, San Antonio, TX;* [3]*Knipling-Bushland U.S. Livestock Insects Research Laboratory, Kerrville, TX*

ThP 234 **Investigating MS with MS: A comprehensive sample preparation for MALDI-TOF MSI of in situ mouse brain lipids.**; Krista A Berlin; *University of Texas in San Antonio, San Antonio, TX*

ThP 235 **DIUTHAME enables matrix-free mass spectrometry imaging of frozen tissue sections of Alzheimer's disease (AD) brain**; Masaya Ikegawa[1]; Yumiko Toyama[2]; Yume Mukasa[2]; Inori Shintani[2]; Takayuki Ohmura[3]; Masahiro Kotani[3]; Akira Tashiro[3]; Takashi Nirasawa[4]; Ryo Kajita[4]; Nobuto Kakuda[2]; Shigeo Murayama[5]; Yasuhide Naito[6]; [1]*Doshisha University, Kyotanabe City, Japan;* [2]*Doshisha University, Kyotanabe, Japan;* [3]*Hamamatsu Photonics K.K., Iwata, Japan;* [4]*Bruker Japan K.K., Yokohama, Japan;* [5]*Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Japan;* [6]*The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan*

ThP 236 **High speed and high resolution mass spectrometry imaging using wide-field sampling**; Xiangyu Guo; *Tsinghua University, Beijing, China*

ThP 237 **AP-MALDI imaging of enzymatic degradation of polysaccharides in maize kernels**; Jonatan Riber Granborg[1]; Svend Kaasgaard[2]; Christian Janfelt[3]; [1]*University of Copenhagen, Novozymes A/S, Kongens Lyngby, Denmark;* [2]*Novozymes A/S, Kgs. Lyngby, Denmark;* [3]*University of Copenhagen, København, Denmark*

ThP 238 **Supermolecule-assisted Imaging of Low-Molecular Weight Quaternary Ammonium Compounds by MALDI-MS of their Non-covalent Complexes with Cucurbit[7]uril**; Di Chen[1, 2]; Jun Han[1, 3]; Juncong Yang[1]; Zhenzhong Zhang[2]; Christoph H. Borchers[1, 4, 5, 6, 7]; [1]*University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC;* [2]*School of Pharmaceutical Sciences, Zhengzhou University, Zhengzhou, China;* [3]*Division of Medical Sciences, University of Victoria, Victoria, BC;* [4]*Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC;* [5]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC;* [6]*Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia;* [7]*Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

ThP 239 **On-Tissue Derivatization for Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging of N-Glycans in Cancer Tissues**; Hua Zhang[1]; Xudong Shi[2]; Nhu Vu[1]; Yatao Shi[1]; Miyang Li[3]; Bin Wang[1]; Lingjun Li[1, 3]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222;* [2]*Department of Surgery, University of Wisconsin-Madison, Madison, WI;* [3]*Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222*

ThP 240   **Development of high sensitivity mass spectrometry imaging based on DIUTHAME chip**; <u>Masahiro Kotani</u>[1]; Takayuki Ohmura[1]; Akira Tashiro[1]; Yasuhide Naito[2]; [1]*HAMAMATSU PHOTONICS K.K., Iwata City, Shizuoka Pref., Japan;* [2]*The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan*

ThP 241   **Combining crown ether host-guest chemistry with mass spectrometry imaging to reveal dynamic sodium and potassium levels in tissue**; <u>Leonidas Mavroudakis</u>[1]; Kyle Daniel Duncan[1]; Ingela Lanekoff[1]; [1]*Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden*

ThP 242   **ToF-SIMS 3D Visualization and Quantification of Particles Embedded in Matrices as Model Systems for Characterization of Oral Drug Delivery Films**; <u>Shin Muramoto</u>; *National Institute of Standards and Technology, Gaithersburg, MD*

ThP 243   **Lipid Analysis using Select Matrices with MALDI-2 Post-ionization for Advanced Imaging Applications**; <u>Josiah C Mcmillen</u>[1,2]; Jarod A. Fincher[2,3]; Jeffrey M Spraggins[1,2,3]; Richard M Caprioli[1,2,3,4,5]; [1]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Department of Pharmacology, Vanderbilt University, Nashville, TN;* [5]*Department of Medicine, Vanderbilt University, Nashville, TN*

ThP 244   **Comparative Analysis and Peptide Maping of Ethanol and Formalin-Fixed Alzheimer's Human Brain Tissue**; <u>Savannah Dyer</u>[1]; Andrea R Kelley[1]; Xiongwei Zhu[2]; George Perry[1]; Stephan B.H. Bach[1]; [1]*The University of Texas at San Antonio, San Antonio, TX;* [2]*Case Western Reserve University, Cleveland, OH*

ThP 245   **On tissue-derivatization of lipopolysaccharide for detection of lipid A using MALDI MSI**; <u>Hyojik Yang</u>[1]; Courtney E Chandler[1]; Francesca M Gardner[1]; David Varisco[1]; David R Goodlett[1,2]; Robert K Ernst[1]; Alison J. Scott[1,3]; [1]*University of Maryland School of Dentistry, Baltimore, MD;* [2]*University of Gdansk, International Center for Cancer Vaccine Science, Gdansk, Poland;* [3]*Maastricht Multimodal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands*

ThP 246   **Advanced Methods for Differentiating Lipid Isomers in Tissue using Trapped Ion Mobility Imaging Mass Spectrometry**; <u>Katerina V Djambazova</u>[1,2]; Lukasz Migas[3]; Dustin Klein[2,4]; Emilio S Rivera[2,4]; Elizabeth Kathleen Neumann[2,4]; Martin Dufresne[4,5]; Raf Van De Plas[3,4,6]; Richard M. Caprioli[1,4,6,7,8]; Jeffrey M Spraggins[1,2,4]; [1]*Vanderbilt University Department of Chemistry, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205;* [3]*Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands;* [4]*Vanderbilt University, Department of Biochemistry, Nashville, TN;* [5]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [6]*Mass Spectrometry Research Center, Nashville, TN;* [7]*Department of Medicine, Vanderbilt University, Nashville, TN;* [8]*Department of Pharmacology, Vanderbilt University, Nashville, TN*

ThP 247   **Towards lipid MALDI-MS imaging in FFPE tissue: antigen retrieval and its effect on positive ion species**; <u>Vanna Denti</u>[1]; Isabella Piga[1]; Sonia Guarnerio[2]; Francesca Clerici[1]; Clizia Chinello[1]; Giuseppe Paglia[1]; Fulvio Magni[1]; Andrew Smith[1]; [1]*Clinical Proteomics and Metabolomics Unit, Department of Medicine and Surgery, University of Milano-Bicocca, Vedano al Lambro, Italy;* [2]*Biomolecular Sciences Research Centre, Sheffield-Hallam University, Sheffield, United Kingdom*

IMAGING MS: PHARMACEUTICALS, METABOLITES, AND LIPIDS II
ThP 248-261

ThP 248   **Mapping Spatial Distributions of Drug Candidates for Inflammatory Bowel Disease with MALDI Mass Spectrometry Imaging**; <u>Meng Xu</u>[1]; Dylan Nicholas Tabang[1]; Bing Tian[2]; Allan R Brasier[3]; Jia Zhou[2]; Lingjun Li[1,4]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222;* [2]*University of Texas Medical Branch at Galveston, Galveston, TX;* [3]*University of Wisconsin-Madison, Madison, Wisconsin;* [4]*School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222*

ThP 249   **Mass Spectrometry and Immunofluorescence Imaging to Identify Markers of Treatment Response to Anti-PD1 in Syngeneic Tumor Models**; <u>Mary King</u>[1]; Robert Yuan[2]; Jeremy Chen[2]; Isabel Sariol[1]; Shirley Li[1]; Oscar Ekpenyong[2]; Janica Wong[2]; Jennifer Yearley[2]; Luis Zúñiga[2]; Maribel Beaumont[2]; Jin-Hwan Han[2]; Livia S Eberlin[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*Merck & Co., Kenilworth, NJ*

ThP 250   **Cutaneous drug delivery of tofacitinib in vehicles containing dexpanthenol or sodium lauryl sulphate**; <u>Anne Mette Handler</u>[1,2]; Mariam Fallah[1,2]; Gitte Pommergaard Pedersen[2]; Kim Troensegaard Nielsen[2]; Christian Janfelt[1]; [1]*University of Copenhagen, Copenhagen, Denmark;* [2]*LEO Pharma A/S, Ballerup, Denmark*

ThP 251   **Spatial metabolomics to trace metabolic deregulation and pathological heterogeneity in MYC-driven mammary gland tumours**; <u>Adam J Taylor</u>[1]; Avinash Ghanate[2]; Peter Kreuzaler[2]; Yulia Panina[2]; Spencer A Thomas[1]; Alex Dexter[1]; Alejandro Suarez-Bonnet[3]; Simon L Priestnall[3]; Ian S Gilmore[1]; Greg Mcmahon[1]; Zoltan Takats[4]; Mariia Yuneva[2]; Josephine Bunch[1,4]; [1]*National Physical Laboratory, Teddington, United Kingdom;* [2]*The Francis Crick Institute, London, United Kingdom;* [3]*The Royal Veterinary College, North Mymms, United Kingdom;* [4]*Imperial College London, London, United Kingdom*

ThP 252 **Identification of phosphonolipids and spatial distribution in tissues of marine bivalves**; Patric Bourceau[1]; Benedikt Geier[1]; Dolma Michellod[1]; Manuel Liebeke[1]; [1]*Max Planck Institute for Marine Microbiology, Bremen, Germany*

ThP 253 **Low abundant metabolites/oxidized lipids imaging in single cells undergoing ferroptosis using H2O gas cluster ion beam secondary ion mass spectrometry(H--2O-GCIB-SIMS)**; Hua Tian[1, 2]; Louis J. Sparvero[3, 4]; Andrew A. Amoscato[3, 4]; Valerian E. Kagan[3, 4, 5]; Hülya Bayır[3, 4, 5]; Nicholas Winograd[1]; [1]*Department of Chemistry, Pennsylvania State University, University Park, PA;* [2]*Materials Research Institute, Pennsylvania State University, University Park, PA;* [3]*Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA;* [4]*Center for Free Radical and Antioxidant Health, University of Pittsburgh, Pittsburgh, PA;* [5]*Department of Critical Care Medicine, and Safar Center for Resuscitation Research, University of Pittsburgh, Pittsburgh, PA*

ThP 254 **Modification of Lipid Expression in AKI kidney and possible reversion with Ferrostatin treatment studied by MLADI-IMS**; Lucia Martín-Saiz[1]; Olatz Fresnedo[2]; Ana Belen Sanz Bartolomé[3]; Jose A Fernández[1]; Alberto Ortiz Arduan[3]; [1]*1Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU),, Leioa, Spain;* [2]*2Department of Physiology, Fac. of Medicine and Nursing, University of the Basque Country(UPV/EHU), Leioa, Spain;* [3]*3Laboratory of Nephrology, IIS-Foundation Jimenez Diaz, Madrid, Spain*

ThP 255 **Spatiotemporal Dynamics of Bioactive Lipids in Arteries Undergoing Restenosis Observed and Identified at High Spatial Resolving Power**; Gregory L Fisher[1]; Yatao Shi[2]; Jillian Johnson[2]; Bowen Wang[3]; Bingming Chen[2]; Go Urabe[3]; Xudong Shi[4]; K. Craig Kent[3]; Lian-Wang Guo[3]; Lingjun Li[2, 5]; [1]*Physical Electronics, Chanhassen, MN;* [2]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [3]*Davis Heart and Lung Research Institute, The Ohio State University, Columbus, Ohio;* [4]*Department of Surgery, University of Wisconsin-Madison, Madison, WI;* [5]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 256 **DESI-MS imaging to visualize the spatial distribution of xenobiotics and endogenous lipids in the skin**; Wei Rao[1]; Susan Slade[1]; Emmanuelle Claude[1]; Emrys Jones[1]; Frédéric Métral[1]; Julie Quartier[2]; Maria Lapteva[2]; Yogeshvar Kalia[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*University of Geneva, Geneva, Switzerland*

ThP 257 **Diagnosing breast cancer in FFPE tissue samples using DESI-MSI**; Olof Gerdur Isberg[1, 2]; Paolo Inglese[2]; Dipa Gurung[2]; Hiromi Kudo[2]; Sigridur Klara Bodvarsdottir[1]; Jon Gunnlaugur Jonasson[3]; Margret Thorsteinsdottir[1]; Zoltan Takats[2]; [1]*University of Iceland, Reykjavik, Iceland;* [2]*Imperial College London, London, United Kingdom;* [3]*Landspitali -The National University Hospital of Iceland, Reykjavik, Iceland*

ThP 258 **Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS) subcellular imaging of low abundance phosphatidylethanolamine metabolites in traumatized brain neurons**; L.j. Sparvero[1]; Hua Tian[2]; Wanyang Sun[1]; Andrew A. Amoscato[1]; Simon C. Watkins[1]; Nicholas Winograd[2]; Valerian E. Kagan[1]; Hülya Bayir[1]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*The Pennsylvania State University, University Park, PA*

ThP 259 **MALDI-Imaging Mass Spectrometry of Virgin and Bleached Human Hair: An Analytical Technique to Identify "Moisturized" Hair Biomarkers**; Stella K Betancourt[1]; Yi Fan[1]; Wendy Kin Man Chan[1]; Shouxun Zhao[1]; [1]*BASF, Tarrytown, NY*

ThP 260 **Multi-Modal Mass Spectrometry Imaging of an Animal Model of High-Grade Serous Ovarian Cancer Provides Deeper Coverage**; Clint M. Alfaro[1]; Olga Kim[2]; Eunyoung Park[2]; Jaeyeon Kim[2, 3]; Facundo M. Fernandez[1]; [1]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia;* [2]*Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN;* [3]*Indiana University Melvin & Bren Simon Cancer Center, Indianapolis, IN*

ThP 261 **Metabolomic mapping of mouse thymus with Imaging Mass Microscope as a whole animal model**; Yudai Tsuji[1]; Shinichi Yamaguchi[2]; Takushi Yamamoto[2]; Tomoyuki Nakamura[3]; Masaya Ikegawa[1]; [1]*Doshisha University, Kyotanabe, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan;* [3]*Kansai Medical University, Hirakata, Japan*

**IMAGING MS: SOFTWARE AND COMPUTATIONAL METHODS
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ThP 262 **Investigating the interactions of the first 17 residues of Huntington protein with lipid vesicles using ESI-MS experiments and MD simulations**; Ahmad Kiani Karanji[1]; Maryssa Beasely[1]; Daud Sharif[1]; Ali Ranjbaran[1]; Justin Legleiter[1]; Stephen J Valentine[1]; [1]*West Virginia University, Morgantown, WV*

ThP 263 **Quality assessment of MALDI TOF and ion mobility MSI data based on mass defect and CCS filtering**; Tobias Boskamp[1, 2]; Rita Casadonte[3]; Lena Hauberg-Lotte[2]; Janina Oetjen[1]; Alice Ly[1]; Sören-Oliver Deininger[1]; Jan H. Kobarg[1]; Richard Drake[4]; Jörg Kriegsmann[3]; Peter Maass[2]; Dennis Trede[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*University of Bremen, Bremen, Germany;* [3]*Proteopath GmbH, Trier, Germany;* [4]*Medical University of South Carolina, Charleston, SC*

ThP 264 **Automated feature finding and evaluation of m/z images based on CCS separation in MALDI TIMS imaging data**; Jan H. Kobarg[1]; Janina Oetjen[1]; Annika Koch[1]; Corinna Henkel[1]; Christian Marsching[2]; Andra Pascale[1]; Gabriele Penazzi[1]; Nikolas Kessler[1]; Wiebke Timm[1]; Aiko Barsch[1]; Tobias Boskamp[1]; Heiko Neuweger[1]; Carsten Hopf[2]; Dennis Trede[1]; Sören-Oliver Deininger[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim Technical University, Mannheim, Germany*

ThP 265   **Development of data processing tools for conformational mass spectrometry imaging**; Emma K Sisley[1]; Iain B Styles[1]; Helen J Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

ThP 266   **intact protein mass spectrometry imaging of human non-alcoholic fatty liver disease on an orbitrap eclipse using a cylindrical FAIMS DEVICE**; James W. Hughes[1]; Iain B. Styles[1]; Patricia F. Lalor[1]; Helen J. Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

ThP 267   **A multi-layered desorption electrospray ionisation (DESI) mass spectrometry imaging workflow for fully annotated datasets**; Emrys A Jones[1]; Praveen Harapanahalli[1]; Emmy Hoyes[1]; Keith Richardson[1]; Michael Morris[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

ThP 268   **Using high abundance proteins as guides for fast and effective peptide/protein identification from metaproteomic data**; Moses H Stamboulian[1]; Sujun Li[1]; Yuzhen Ye[1]; [1]*Indiana University, Bloomington, IN*

ThP 269   **Feature Engineering Guided by Matrix Effects for Mass Spectrometry Imaging Segmentation and Co-localization**; Hang Hu[1]; Ruichuan Yin[1]; Jyothsna Padmakumar Bindu[1]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN*

ThP 270   **FAIR mass spectrometry imaging data analysis of an urothelial carcinoma dataset in a single open-source platform**; Melanie Christine Föll[1]; Veronika Volkmann[1]; Kathrin Enderle-Ammour[1]; Peter Bronsert[1, 2, 3]; Oliver Schilling[1, 2]; [1]*Institute of Surgical Pathology, Medical Center, Freiburg University, Freiburg, Germany; [2]German Cancer Consortium (DKTK) and Cancer Research Center (DKFZ), Freiburg, Germany; [3]Tumorbank Comprehensive Cancer Center Freiburg, Freiburg, Germany*

ThP 271   **Analysis of Metabolites Relevant to Growth of Retinal Blood Vessels using the Single-probe MS Imaging Combined with Fluorescence Microscopy**; Zhu Zou[1]; Pengchun Yu[2]; Xiang Tian[3]; Jie Zhu[2]; Zhibo Yang[1]; [1]*University of Oklahoma, Norman, OK; [2]Oklahoma Medical Research Foundation, Oklahoma City, OK; [3]Astrazeneca, Gaithersburg, MD*

ThP 272   **Structure-preserving and perceptually-consistent approach for visualization of mass-spectrometric imaging datasets**; Anastasia Sarycheva[1]; Anton Grigoryev[1, 2]; Dmitry Sidorchuk[2]; Gleb Vladimirov[1]; Yury Kostyukevich[1]; Eugene (evgeny) Nikolaev[1]; [1]*Skolkovo institute of science and technology, Moscow, Russia; [2]Kharkevich Institute for Information Transmission Problems, Russian Academy of Sciences, Moscow, Russia*

ThP 273   **Spatially-aware clustering of ion images in mass spectrometry imaging data through use of pre-trained neural networks**; Wanqiu Zhang[1, 2]; Nico Verbeeck[1, 2]; Thomas Moerman[2]; Etienne Waelkens[3]; Marc Claesen[1, 2]; Bart De Moor[1]; [1]*KU Leuven, ESAT-STADIUS, Leuven, Belgium; [2]Aspect Analytics NV, Genk, Belgium; [3]KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium*

ThP 274   **Deep multiple instance learning classifies subtissue locations in mass spectrometry images from tissue-level annotations**; Dan Guo[1]; Melanie Christine Föll[2]; Veronika Volkmann[2]; Kathrin Enderle-Ammour[2]; Peter Bronsert[2, 3]; Oliver Schilling[2]; Olga Vitek[1]; [1]*Northeastern University, Boston, MA; [2]University of Freiburg, Freiburg, Germany; [3]German Cancer Consortium (DKTK) and Cancer Research Center (DKFZ), Freiburg, Germany*

ThP 275   **Utility of principal component analysis plots for optimizing AuNPs for Mass Spectrometry Imaging**; Cameron Shedlock[1]; Tyler Bielinski[1]; Nolan K Mclaughlin[1]; Jason Graham[1]; Katherine A. Stumpo[1]; [1]*University of Scranton, Scranton, PA*

ThP 276   **Towards nanoscale molecular mass spectrometry imaging via physically constrained machine learning on coregistered multimodal data**; Nickolay Borodinov[1]; Matthias Lorenz[1, 2]; Dustin Klein[3, 4]; Jeffrey M Spraggins[3, 4, 5]; Anton Ievlev[1]; Olga S. Ovchinnikova[1]; [1]*Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; [2]University of Tennessee Knoxville, Knoxville, TN; [3]Vanderbilt University, Department of Biochemistry, Nashville, TN; [4]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; [5]Vanderbilt University Department of Chemistry, Nashville, TN*

ThP 277   **Automatic detection and identification of drug metabolites in MSI datasets**; Fabien Pamelard[1]; Anas Carfache[1]; Mathieu Gaudin[1]; Rima Ait Belkacem[1]; David Bonnel[1]; Jonathan Stauber[2]; [1]*ImaBiotech, Loos, France; [2]ImaBiotech, Billerica, Massachusetts*

INFORMATICS: PEPTIDE ID AND QUANTIFICATION
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ThP 278   **Concurrent Glycopeptide Identification from multiple related LC-MS/MS datasets by using spectra clustering**; Rui Zhang[1]; Sujun Li[1]; Lei Wang[1]; Jinghui Zhu[2]; Yehia Mechref[3]; David M Lubman[4]; Haixu Tang[1]; [1]*Indiana University, Bloomington, IN; [2]University of Michigan, School of Medicine, Rogel Cancer Center, Ann Arbor, Michigan; [3]Texas Tech University, Lubbock, Texas; [4]University of Michiagan, Ann Arbor, MI*

ThP 279   **Trypsin - a Tired Workhorse? The Selectivity of Atypical Cleavages by Trypsin**; Meghan Burke[1]; Yuxue Liang[1]; Stephen E. Stein[1]; [1]*National Institute of Standards and Technology, Gaithersburg, Maryland*

ThP 280   **JUMP-batch: A tool to rescue missing peptides and remove batch effects using internal references and linear model fitting**; Suresh Poudel[1]; Yuxin Li[2]; Junmin Peng[2, 3]; [1]*1Departments of Structural Biology and*

Developmental Neurobiology, St. Jude Children's Research Hospital,, Memphis, Tennessee; [2]Center for Proteomics and Metabolomics, St. Jude Children's Research Hospital, Memphis, TN; [3]Departments of Structural Biology and Developmental Neurobiology, St. Jude Children's Research Hospital, Memphis, TN

ThP 281 **Breaking the logjam: fast peptide identification and quantification in timsTOF PASEF data**; Fengchao Yu[1]; Sarah E. Haynes[1]; Guo Ci Teo[1]; Dmitry M. Avtonomov[1]; Andy T. Kong[1]; Felipe Da Veiga Leprevost[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 282 **PASER: Parallel Database Search Engine in Real-Time**; Robin Park[1]; Patrick Garrett[1]; Michael Krause[2]; Sven Brehmer[2]; Titus Jung[1]; Peter Huffnagel[2]; Christopher Adams[2]; Casimir Bamberger[1]; Jolene Diedrich[1]; John Robert Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Bruker, Bremen, Germany*

ThP 283 **An extension of Mass++ ver.4, a data viewer, for proteome analysis**; Satoshi Tanaka[1]; Masaki Murase[2]; Masaki Kato[2]; Tsuyoshi Tabata[2]; Maiko Kusano[3]; Shin Kawano[4]; Susumu Goto[5]; Yasushi Ishihama[2]; Akiyasu C. Yoshizawa[2]; *[1]Trans-IT, Kaminokawa-machi, Tochigi Pref., Japan; [2]Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; [3]Res. Inst. of Environ. Med., Nagoya Univ., Nagoya, Japan; [4]Toyama Intl. Univ., Toyama, Japan; [5]DBCLS, DS, ROIS, Kashiwa, Japan*

ThP 284 **A Machine-Learning-Combined Scoring Method for Peptide Feature Detection from LC-MS**; Xiangyuan Zeng[1]; Bin Ma[1]; Shenheng Guan[2]; *[1]University of Waterloo, Waterloo, ON; [2]University of California, Los Angeles, Los Angeles, CA*

ThP 286 **PointNovo: instrument-resolution-independent de novo peptide sequencing with deep learning**; Rui Qiao[1]; Ngoc Hieu Tran[2]; Lei Xin[2]; Xin Chen[2]; Baozhen Shan[2]; Ming Li[1]; Ali Ghodsi[1]; *[1]University of Waterloo, Waterloo, ON; [2]Bioinformatic Solutions Incorporation, Waterloo, Ontario*

ThP 287 **Machine learning-based spectral filtering tool for processing peptide mass spectra**; Krishna Anapindi[1, 2]; Yuxuan Xie[1, 2]; Jonathan V Sweedler[1, 2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]Beckman Institute, Urbana, IL*

ThP 288 **Deep learning-derived evaluation metrics for benchmarking computational pipelines for the analysis of large-scale phosphoproteomics datasets**; Wen Jiang[1]; Kai Li[1]; Bo Wen[1]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 289 **Rapid Total Search: Peptide Identification in 200 Million Proteins with Unrestricted Modifications and Nonspecific Digestion**; Qixin Liu[1]; Noah Reinhardt[2]; Bin Ma[3]; *[1]Rapid Novor inc, Kitchener, ON; [2]Rapid Novor Inc, Waterloo, ON; [3]University of Waterloo, Waterloo, ON*

ThP 290 **PASEF and Bolt: enabling comprehensive analysis via high MS/MS acquisition speed and MS/MS sequencing through vast protein databases in minutes**; Amol Prakash[1]; Swetaketu Majumder[1]; Jiefei Tong[2]; Shenheng Guan[3]; Matt Willetts[4]; Bin Ma[3]; Tharan Srikumar[5]; Michael F. Moran[2]; *[1]Optys Tech Corporation, Shrewsbury, MA; [2]Sick Kids Research Center, Toronto, M5G1X8; [3]University of Waterloo, Waterloo, ON; [4]Bruker Scientific LLC, Billerica, MA; [5]Bruker Ltd, Milton, L9T 6P4*

ThP 291 **Filtering and optimization of peptide tandem mass spectral libraries**; Sergey Sheetlin[1]; Guanghui Wang[1]; Dmitrii V. Tchekhovskoi[1]; Zheng Zhang[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 292 **A proteogenomics pipeline for identifying sample-specific proteoforms by combining RNA-Seq and top-down mass spectrometry**; Wenrong Chen[1]; Xiaowen Liu[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

ThP 293 **MS Amanda goes West: Integrating a search engine into Skyline**; Viktoria Dorfer[1]; Marina Strobl[1]; Nicholas Shulman[2]; Matthew C Chambers[2]; Michael J MacCoss[2]; Brendan Maclean[2]; *[1]Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria; [2]Department of Genome Sciences, University of Washington, Seattle, WA*

ThP 294 **Separating the wheat from the chaff: Prediction-assisted rescoring**; Siegfried Gessulat[1]; Tobias Schmidt[2]; Michael Graber[1]; Florian Seefried[1]; Carmen Paschke[3]; Kai Fritzemeier[3]; David M Horn[4]; Bernard Delanghe[3]; Daniel P Zolg[2]; Mathias Wilhelm[2]; Bernhard Kuster[2]; Martin Heinrich Frejno[1]; *[1]msAId GmbH, Garching, Germany; [2]TU Munich, Freising, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]ThermoFisher Scientific, San Jose, CA*

ThP 295 **The good, the bad and the ugly: Peptide IDs you will encounter**; Siegfried Gessulat[1]; Tobias Schmidt[2]; Michael Graber[1]; Florian Seefried[1]; David M Horn[3]; Bernard Delanghe[4]; Daniel P Zolg[2]; Mathias Wilhelm[2]; Bernhard Kuster[2]; Martin Heinrich Frejno[1]; *[1]msAId GmbH, Garching, Germany; [2]TU Munich, Freising, Germany; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 296 **Comprehensive analysis of the intermolecular associations of peanut proteins by SEC coupled with offline bottom-up MS**; Abigail S Burrows[1]; Justin T Marsh[1]; Philip E Johnson[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

ThP 297   **A new algorithm for HDMSE data analysis with deep proteome coverage**; Zia Rahman[1]; Leroy B Martin Iii[2]; Susan Slade[3]; Di Wang[1]; Weiwu Chen[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON; [2]Waters Corporation, Milford, Massachusetts; [3]Waters Corporation, Wilmslow, United Kingdom*

ThP 298   **Identifying genetically variant peptides in cancer samples by the NIST hybrid spectral library search**; Guanghui Wang[1]; Meghan C. Burke[1]; Sergey L. Sheetlin[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 299   **Interactive Spectrum Validator as an inter-resource tool for fragment ion spectrum comparison between experimental and (predicted) reference spectra**; Tobias Schmidt[1]; Patroklos Samaras[1]; Viktoria Dorfer[2]; Christian Panse[3]; Tobias Kockmann[3]; Leon Bichmann[4]; Bart Van Puyvelde[5]; Yasset Perez-Riverol[6]; Eric W. Deutsch[7]; Wout Bittremieux[8]; Bernhard Kuster[1]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria; [3]Functional Genomics Center (ETH), Zurich, Switzerland; [4]Applied Bioinformatics, Tübingen, Germany; [5]Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium; [6]European Molecular Biology Laboratory , European Bioinformatics Institute (EMBL-EBI), Hinxton, United Kingdom; [7]Institute For Systems Biology, Seattle, WA; [8]University of California San Diego, San Diego, La Jolla, California*

ThP 300   **A Strategy for Discovery of Public Tumor-Associated HLA Antigens Using MetaMorpheus**; Isabella T Whitworth[1]; Katherine B Henke[1]; Robert J Millikin[1]; Hemanth Potluri[2]; Mark Scalf[1]; Brian L Frey[1]; Michael R. Shortreed[1]; Douglas G Mcneel[3]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin; [2]University of Wisconsin School of Medicine and Public Health, Madison, WI; [3]University of Wisconsin Carbone Cancer Center, Madison, WI*

ThP 301   **Restricting classifier training datasets improves error rate estimation when searching highly-specific libraries**; Seth Just[1]; Brendan Maclean[2]; Lukas Käll[3]; Hannes Röst[4]; Brian Searle[1, 5]; *[1]Proteome Software, Portland, OR; [2]University of Washington, Seattle, WA; [3]Royal Institute of Technology - KTH, Solna, Sweden; [4]University of Toronto, Toronto, ON; [5]Institute for Systems Biology, Seattle, WA*

ThP 302   **An automated, accessible proteogenomic pipeline for high confidence detection and rigorous validation of novel peptide sequence variants in Galaxy-P**; Andrew T. Rajczewski[1]; Bo Wen[2]; James E. Johnson[1]; Ray Sajulga[1]; Qiyuan Han[1]; Praveen Kumar[1]; Pratik Dilip Jagtap[1]; Bing Zhang[2]; Natalia Tretyakova[1]; Timothy J Griffin[1]; *[1]University of Minnesota at Twin Cities, Minneapolis, MN; [2]Baylor College of Medicine, Houston, TX*

ThP 303   **Quality Control of Results from Searchable Spectral Archive**; Long Wu[1]; Henry Lam[1]; *[1]The Hong Kong University of Science and Technology, Kowloon, Hong Kong*

ThP 304   **Maestro Merge: Expedited and thorough peptide analysis of large-scale, multiple-condition datasets**; Julie Wertz[1]; Nuno Bandeira[1]; *[1]University of California San Diego, San Diego, CA*

ThP 305   **A Fast and Accurate Proteomic Search Engine Utilizing A Precalculated Fragmentation Database**; Jeffrey J. Jones; *SoCal Bioinformatics Inc., Montrose, CA*

ThP 306   **Cancer neoantigen prioritization through sensitive and reliable proteogenomics analysis**; Bo Wen[1]; Kai Li[1]; Yun Zhang[1]; Bing Zhang[1]; *[1]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX*

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ThP 307   **Clustering of label-free quantification data: a quantification-first approach**; Matthew The[1, 2]; Lukas Käll[1]; *[1]Royal Institute of Technology - KTH, Solna, Sweden; [2]TU Munich, Munich, Germany*

ThP 308   **New functionality for the Trans-Proteomic Pipeline: tools for the analysis of proteomics data**; Luis Mendoza[1]; David Shteynberg[1]; Michael Hoopmann[1]; Henry Lam[2]; Jimmy K Eng[3]; Eric W. Deutsch[1]; Robert L. Moritz[1]; *[1]Institute For Systems Biology, Seattle, WA; [2]Hong Kong University of Science and Technology, Hong Kong, China; [3]University of Washington, Seattle, WA*

ThP 309   **Compliant-Ready Intact Biotherapeutic Protein Quantitation Using Reconstructed Masses**; Kerstin Pohl[1]; Wenying Jian[2]; Naidong Weng[2]; Yihan Li[3]; Ji Jiang[3]; Xu Guo[4]; Vanaja Raguvaran[4]; Lei Xiong[3]; *[1]Sciex, Framingham, MA; [2]Janssen R&D LLC., Spring House, PA; [3]SCIEX, Redwood Shores, CA; [4]SCIEX, Concord, ON*

ThP 310   **Search Compare Cache Files and the Raw Data Extraction Daemon Improve Quantification Analysis Support and Ease of Protein Prospector Installation**; Peter R Baker[1]; Juan A. Oses[2]; Bing Gao[2]; Robert J. Chalkley[2]; *[1]UCSF, Rokietnica, Poland; [2]UCSF, San Francisco, CA*

ThP 311   **Proteomic analysis of multiple neuroanatomical regions of Normal Human Brain: a database and community resource for neuroscience research**; Deeptarup Biswas[1]; Chetanya Gupta[1]; Sanjyot Shenoy[1]; P. Athithyan[1]; Susmita Ghosh[1]; Sudesh Roy[1]; Sanjeeva Srivastava[1]; *[1]IIT Bombay, Mumbai, India*

ThP 313   **Proceed with caution: Considerations for Protein Inference and Quantitation in Metaproteomics**; Samantha L. Peters[1, 2]; Payal Chirania[1, 2]; Paul E. Abraham[1, 2]; Richard J. Giannone[1, 2]; Robert L. Hettich[1, 2]; *[1]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; [2]University of Tennessee Knoxville, Knoxville, TN*

ThP 314   **TMT-Pro 16-plex labeling and unsupervised clustering for analysis of organellar proteome dynamics**; <u>Nicholas Carruthers</u>[1]; Kezhong Zhang[1]; Paul M. Stemmer[1]; [1]*Wayne State University, Detroit, MI*

ThP 315   **De Novo Sequencing with Twister: Expanding Opportunities**; <u>Kira Vyatkina</u>; *Alferov University, St Petersburg, Russia*

ThP 316   **Integration of MSstatsTMT into Proteome Discoverer using the Scripting Node**; <u>David M. Horn</u>[1]; Ting Huang[2]; Meena Choi[2]; Olga Vitek[2]; Rosa I. Viner[1]; Frank Berg[3]; Kai Fritzemeier[3]; Carmen Paschke[3]; [1]*Thermo Fisher Scientific, San Jose, CA; [2]Northeastern University, Boston, MA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 317   **Updates to FragPipe: from LC-MS data to protein identifications, quantification, and PTM localization in just a few clicks**; Dmitry Avtonomov[1]; Fengchao Yu[1]; Guo Ci Teo[1]; Felipe Da Veiga Leprevost[1]; Sarah E. Haynes[1]; Hui-Yin Chang[1]; Daniel J. Geiszler[1]; Daniel A. Polasky[1]; <u>Alexey I. Nesvizhskii</u>[1]; [1]*University of Michigan, Ann Arbor, MI*

ThP 318   **A Bayesian Null Interval Hypothesis Test Controls False Discovery Rates and Improves Sensitivity in Label-Free Quantitative Proteomics**; <u>Robert Millikin</u>[1]; Michael R. Shortreed[1]; Mark Scalf[1]; Lloyd M. Smith[1]; [1]*University of Wisconsin Madison, Madison, WI*

ThP 319   **A new algorithm for FAIMS data analysis with accurate in-depth quantitative profiling**; Zia Rahman[1]; Yandong Zhu[2]; Kassim Santone[2]; Zheng Chen[2]; Bernard Delanghe[3]; <u>Baozhen Shan</u>[2]; [1]*Bioinformatics Solutions Inc, Waterloo, ON; [2]Bioinformatics Solutions Inc., Waterloo, ON; [3]Thermo Fisher Scientific, Cambridge, MA*

ThP 320   **MealTime-MS: A machine learning-guided real-time mass spectrometry analysis for protein identification and efficient dynamic exclusion**; <u>Yun-En Chung</u>[1]; Alexander R. Pelletier[1]; Zhibin Ning[1]; Nora Wong[1]; Daniel Figeys[1]; Mathieu Lavallée-Adam[1]; [1]*University of Ottawa, Ottawa, ON*

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ThP 321   **A fast ultra-low noise current amplifier with linear dynamic range from femtoamperes to nanoamperes**; <u>Ansgar T. Kirk</u>[1]; Cornelius Wendt[1]; Stefan Zimmermann[1]; [1]*Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Hannover, Germany*

ThP 322   **Anatomy of Protein ESI Mass Spectra by Superconducting Tunnel Junction Mass Spectrometry**; <u>Li-Xue Jiang</u>[1]; Mark E. Bier[1]; [1]*Carnegie Mellon University, Pittsburgh, PA*

ThP 323   **A Discrete-Dynode Detector for Quadrupole RGA Applications**; <u>Aditya Wakhle</u>[1]; Peter Raffin[1]; Sid Sondur[1]; Toby Shanley[1]; Scott Morgan[1]; [1]*Adaptas Solutions, Sydney, Australia*

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS
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ThP 324   **A Robust C-Trap Ion Injection Method Incorporating Electrodynamic Squeezing**; <u>Hamish Stewart</u>[1]; Ralf Hartmer[1]; Christian Hock[1]; Amelia Peterson[1]; Eric Wapelhorst[1]; Alexander Makarov[1]; [1]*Thermo Fisher Scientific, Bremen, Germany*

ThP 325   **Increasing the resolving power in a High Field Cassinian ion trap**; <u>Björn Raupers</u>[1]; Hana Medhat[2]; Frank Gunzer[2]; Tassilo Muskat[1]; Jurgen Grotemeyer[1]; [1]*Christian-Albrechts-Univ, Kiel, Germany; [2]German University in Cairo, Cairo, Egypt*

ThP 326   **The Case for Development of the Digital Quadrupole Time-of-Flight Mass Spectrometer for High m/z Analysis**; <u>Peter T. A. Reilly</u>[1]; Adam P. Huntley[1]; Margaret E. Reece[1]; [1]*Washington State University, Pullman, WA*

ThP 327   **From m/z to m/µ: The determination of isomer dipole moments and shape with a miniaturized Stark quadrupole mass spectrometer**; John Bracewell[1]; <u>Liam Duffy</u>[1]; [1]*University of North Carolina Greensboro, Greensboro, NC*

ThP 328   **Electrospray Ionization Time-of-Flight Mass Spectrometry Using Constant Momentum Acceleration**; <u>Christopher J Brais</u>[1]; Eric T Jensen[1]; Steven J Ray[1]; [1]*University at Buffalo, SUNY, Buffalo, NY*

ThP 329   **Combinatorial improvement in spectral acquisition rates with harmonic signal and MS array ICR detectors**; <u>Sung-Gun Park</u>[1]; Jared P. Mohr[1]; Gordon A. Anderson[2]; James E Bruce[1]; [1]*University of Washington, Seattle, WA; [2]GAA Custom Engineering, LLC,, Benton, WA*

ThP 330   **Innovations in MS-MS: Development of a Versatile Q-ToF Molecular Beam Mass Spectrometer**; <u>Greg Thier</u>[1]; Steven M Rowland[2]; Brian Regel[1]; [1]*Extrel CMS, Pittsburgh, PA; [2]National Renewable Energy Laboratory, Golden, CO*

ION MOBILITY: APPLICATIONS II
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ThP 331 **Ion Mobility-Mass Spectrometry and Ozone-Induced Cleavage of Endocyclic C=C Bonds to Separate Isomeric Prostaglandins**; Kristie Baker[1]; Samuel W Maddox[1]; Robert H Fraser-Caris[1]; Christopher D. Chouinard[1]; [1]*Florida Institute Of Technology, Melbourne, FL*

ThP 332 **Absolutequantificationof proteins by electrospray-differential mobility analysis- condensation particle counter**; Wei Mi[1]; Zhishang Hu[1]; Yang Liu[2]; [1]*National institute of metrology,China, Beijing, China;* [2]*Beijing University of Chemical Technology, Beijing, China*

ThP 333 **Human cerebrospinal fluid: a comprehensive analysis of glycolipid expression and structure by ion mobility mass spectrometry**; Mirela Sarbu[1]; Vukelic Zeljka[1]; David E. Clemmer[2]; Alina D. Zamfir[3]; [1]*National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania, Timisoara, Romania;* [2]*Indiana University, Bloomington, IN;* [3]*Nat'l Inst, Electrochemistry & Condensed Matter, Timisoara, Romania*

ThP 334 **Identification and Localization of Isomers in Eye Lens Crystallin Peptides Using TWIM-MS**; Hoi Ting Wu[1]; Ryan R. Julian[1]; [1]*University of California, Riverside, Riverside, CA*

ThP 335 **D-amino acid-containing peptide-protein interactions revealed by ion mobility-mass spectrometry (IM-MS) and surface plasmon resonance (SPR)**; Jiabao Guo[1]; Gonyu Li[1]; Lingjun Li[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin*

ThP 336 **A Multiplexed Charge State, m/z Selected, Collision-Induced Unfolding (CIU) Workflow with Pre or Post Quadrupole Activation Using a Q-IMS-ToF Platform**; Martin Green[1]; Keith Richardson[1]; Brandon T. Ruotolo[2]; Daniel A. Polasky[2]; Heidi Gastall[1]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*University of Michigan, Ann Arbor*

ThP 337 **Utilizing U-Shaped Mobility Analyzer (UMA) for High Performance Bio-molecular Analysis**; Ran Qiu[1]; Keke Wang[1]; Xiaoqiang Zhang[1]; Wenjian Sun[1]; [1]*Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China*

ThP 338 **Deep dive into timsTOF data with MSFragger**; Sarah E. Haynes[1]; Fengchao Yu[1]; Guo Ci Teo[1]; Felipe Da Veiga Leprevost[1]; Dmitry M. Avtonomov[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

ThP 339 **Post-ionization mobility separation for MALDI based analysis of isomeric cannabinoids in plant samples**; Arne Behrens[1]; Corinna Henkel[2]; Uwe Karst[1]; [1]*Westfälische Wilhelms-Universität Münster, Münster, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

ThP 340 **A Novel In-Source Ion Fragmentation Device for Comprehensive Small Molecule Analysis by Collision-Induced Dissociation-Ion Mobility-Mass Spectrometry**; Andrzej Balinski[1]; Jaqueline A. Picache[1]; Ruwan T. Kurulugama[2]; Emanuel Zlibut[1]; Jody C. May[1]; John C. Fjeldsted[2]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*Agilent Technologies, Santa Clara, CA*

ThP 341 **Structural Differentiation of Buspirone Hydroxy Metabolites with Cyclic Ion Mobility Spectrometry**; Lauren Mullin[1]; Mark D. Wrona[1]; Martin Palmer[2]; Emma Marsden-Edwards[2]; Robert Plumb[1]; [1]*Waters Corporation, Milford, Massachusetts;* [2]*Waters Corporation, Wilmslow, United Kingdom*

ThP 342 **Structural Analysis of the Glycoprotein Complex Avidin by Tandem-Trapped Ion Mobility Spectrome**; Fanny C. Liu[1]; Tyler C Cropley[1]; Valentina R. Angarita[1]; Wessley Ferguson[1]; Mark E. Ridgeway[2]; Melvin A. Park[2]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL;* [2]*Bruker Daltonics, Billerica, MA*

ThP 343 **Ion mobility separation in a TIMS-TOF PASEF acquisition method decreases spectral complexity**; Joshua Charkow[1]; Annie Ha[1]; Tom W Ouellette[1]; Aparna Srinivasan[1]; Hannes Rost[1]; [1]*University of Toronto, Toronto, ON*

ThP 344 **Characterization of API impurities and degradation products by ion mobility LC-timsTOF Pro with parallel accumulation serial fragmentation (PASEF)**; Zuyun (joel) Huang[1]; Lilly Huang[1]; Song Sun[1]; Xuejun Peng[2]; [1]*SYN Pharmatech, Guelph, ON;* [2]*Bruker Daltonics Inc., San Jose, CA*

ThP 345 **The Potential of Cyclic-Ion Mobility-Mass Spectrometry for the Separation of Steroid Isomers: Application in Food Fraud and Safety**; Eleanor Riches[1]; Nicola Dreolin[1]; Maykel Hernandez-Mesa[2]; Gaud Dervilly[2]; Bruno Le Bizec[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*LABERCA Oniris INRAE, Nantes, France*

ThP 346 **Cyclic ion mobility-mass spectrometry (cIMS) deciphers disulphide bridge pairing in Complementary-Determining Regions (CDRs) of an IgG4 monoclonal antibody**; Hélène Diemer[1]; Thomas Botzanowski[1]; Dale Cooper-Shepherd[2]; Elsa Wagner-Rousset[3]; Evolène Deslignière[1]; Olivier Colas[3]; Guillaume Béchade[2]; Oscar Hernandez-Alba[1]; Alain Beck[3]; Sarah Cianférani[1]; [1]*Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France;* [2]*Waters Corporation, Wilmslow, United Kingdom;* [3]*IRPF - Centre d'Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France*

ThP 347 **Comparison of ion mobility mass spectrometry using direct injections or chromatography in quantitative metabolomics of Rooibos and Honey bush tea**; Maria A Stander[1]; Keabetswe Masike[2]; Dalene De Beer[3, 4]; Andre De Villiers[5]; [1]*Stellenbosch University, Stellenbosch, South Africa;* [2]*Stellenbosch University, Department of Biochemistry, Stellenbosch, South Africa;* [3]*ARC Infruitec-Nietvoorbij, Stellenbosch, South Africa;* [4]*Stellenbosch*

University, Stellenbosch, South Africa; [5]Stellenbosch University, Department of Chemistry, Stellenbosch, South Africa

ThP 348 **A high-throughput differential mobility separation–tandem mass spectrometry (DMS-MS) method for urinary drug testing**; Shirin Hooshfar[1]; Kara L Lynch[1]; [1]*Department of Laboratory Medicine, University of California San Francisco, San Francisco, CA*

ThP 349 **Rapid "Shotgun" APGC-IM-MS Identification and Quantitation of Beta-Sitosterol and Other Phytosterols in Health Supplements**; Jeffrey Morre[1]; Rony Koluda[1]; Dr. Claudia Susanne Maier[1]; [1]*Oregon State University, Corvallis, OR*

ThP 350 **Profiling of the Known-Unknowns Passiflora Complement by Liquid Chromatography - Ion Mobility - Mass Spectrometry**; Michael Mccullagh[1]; Jeff Goshawk[1]; Russell J Mortishire-Smith[1]; Cintia AM Pereira[2]; Janete H Yariwak[3]; Johannes P.C. Vissers[1]; [1]*Waters Corporation, Wilmslow, United Kingdom; [2]Unicep - Centro Universitário Central Paulista, São Carlos, Brazil; [3]Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, Brazil*

LIPIDS: TARGETED AND QUANTITATIVE ANALYSIS
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ThP 351   **Zwitterionic HILIC chromatography - tandem mass spectrometry quantification of acyl carnitines and lysophosphatidic acids: Key metabolites in lipid metabolism**; Natalie Daurio[1]; Kathleen Smith[1]; David Beebe[1]; Kenneth Kelly[1]; Gang Xing[1]; Trenton Ross[1]; Min Wan[1]; Michelle Clasquin[1]; [1]*Pfizer, Cambridge, MA*

ThP 352   **Quantitative Analysis of Cardiolipins by Tandem LC/MS**; Chenchen He[1]; Thekkelnaycke M. Rajendiran[2]; Subramaniam Pennathur[1]; [1]*University of Michigan, School of Medicine, Internal Medicine – Nephrology, Ann Arbor, Michigan;* [2]*University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan*

ThP 353   **A combined direct infusion/ RP-LC-HRMS workflow for accurate absolute quantification with 13C- internal standards for a high number of lipids**; Harald Schoeny[1]; Evelyn Rampler[1, 2, 3]; Felina Hildebrand[1]; Olivia Zach[1]; Gerrit Hermann[1, 4]; Gunda Koellensperger[1, 2, 3]; [1]*University of Vienna, Department of Analytical Chemistry, Vienna, Austria;* [2]*Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria;* [3]*Chemistry meets Microbiology, University of Vienna, Vienna, Austria;* [4]*ISOtopic Solutions, Vienna, Austria*

ThP 354   **The Blood Plasma Lipidome: distinct molecular signatures delineate metabolic health and perturbations in a cross-sectional human cohort**; Si Wu[1]; Daniel Hornburg[1]; Gavin McAllister Traber[1]; Baolong Su[2]; Tejaswini Mishra[1]; Wenyu Zhou[1]; Kevin Contrepois[1]; Sophia Miryam Schüssler-Fiorenza Rose[1]; Monika Avina[1]; Kevin Williams[2]; Michael Snyder[1]; [1]*Stanford University, Palo Alto, CA;* [2]*UCLA, Los Angeles, CA*

ThP 355   **Lipidome-specific features of matrix-bound nanovesicles define their anti-inflammatory and macrophage M2-polarization capacities**; Yulia Tyurina[1]; Vladimir A Tyurin[1]; George S Hussey[1]; Madeline C Cramer[1]; Peter S Timashev[2]; Stephen F Badylak[1]; Valerian E Kagan[1]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*IM Sechenov Moscow State Medical University, Moscow, Russia*

ThP 357   **LC-MS based de-coding of aberrant PMN-MDSC lipidome in cancer: role of FATP-2-triggered signaling**; Vladimir A. Tyurin[1]; Filippo Veglia[2]; Dmitry I. Gabrilovich[2]; Valerian E. Kagan[1]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*The Wistar Institute, Philadelphia, PA*

ThP 358   **Stearoyl CoA desaturase regulates the composition of lipid C=C location isomers**; Simin Cheng[1]; Wenbo Cao[1]; Jiaxin Feng[1]; Qingyuan Hu[1]; Xu Zhao[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; [1]*Tsinghua University, Beijing, China*

ThP 359   **Accumulation of Lysophospholipids in DDE/Dieldrin Treated Largemouth Bass (Micropterus salmoides) Liver Quantified by Targeted Mass Spectrometry**; Mohammad-Zaman Nouri[1]; Kevin Kroll[1]; Nancy Denslow[1]; [1]*University of Florida, Gainesville, FL*

ThP 360   **Rapid and quantification of phospholipid molecular species in plasma based on magnetic solid-phase extraction by MnFe2O4 nanoparticles coupled with LC-HR/MS/MS**; Maw-Rong Lee[1]; Yu-Min Liu[1]; Yen-Hsien Li[1]; [1]*National Chung-Hsing University, Taichung, Taiwan*

ThP 361   **Genome-wide study of the human lipidome and links to cardiovascular disease risk**; Corey Giles[1]; Gemma Cadby[2, 3]; Kevin Huynh[1]; Natalie A Mellett[1]; Gavriel Olshansky[1]; Alexander Smith[1]; Anh Nguyen[1]; Michael Inouye[1]; Eric K Moses[2, 4]; Peter J Meikle[1]; [1]*Baker Heart and Diabetes Institute, Melbourne, Australia;* [2]*Centre for Genetic Origins of Health and Disease, Curtin University and University of Western Australia, Perth, Australia;* [3]*School of Population and Global Health, University of Western Australia, Perth, Australia;* [4]*Menzies Institute for Medical Research, University of Tasmania, Hobart, Australia*

ThP 362   **Method development of high-throughput eicosanoid profiling for micro-sampling plasma**; Masaki Yamada[1]; Naoko Nagano[1]; Tatsuro Nakamura[2]; Takahisa Murata[2]; Takanari Hattori[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*The University of Tokyo, Bunkyo-ku, Japan*

ThP 363   **A validated multiplexed quantitative global molecular lipidomics method with extended coverage for routine use**; Rena N Zhang[1]; Nathan Hatcher[1]; Komal Kedia[1]; Daniel Spellman[1]; Kevin P. Bateman[1]; Kim Ekroos[2]; [1]*Merck & Co., Inc., West Point, PA;* [2]*Lipidomics Consulting Ltd, Esbo, Finland*

ThP 364   **Sensitive and Comprehensive Lipid Mediator Analysis using Advanced Scheduled MRM with Polarity Switching and QTRAP Enhanced Product Ion Scanning**; Paul C Norris[1]; Santosh Kapil Kumar Gorti[1]; Mackenzie J Pearson[1]; [1]*Sciex, Framingham, MA*

ThP 365   **Investigation of the Sulfo-Phospho-Vanillin Assay to Measure Total Lipid Content for Uniform Loading in Quantitative Lipidomic LC-MS/MS Analyses**; Laura Bailey[1]; Kari Basso[1]; [1]*University of Florida Department of Chemistry, Gainesville, FL*

ThP 366   **Development of Extraction Protocol for Telocinobufagin and Investigation of its Enzymatic Hydrolysis by Paraoxonase-1 using HPLC and MS**; Sabitri Lamichhane[1]; Chrysan Joy Mohammed[2]; David Baliu-Rodriguez[1]; Steven T. Haller[1]; David J. Kennedy[1]; Dragan Isailovic[1]; [1]*University of Toledo, Toledo, OH;* [2]*University of Toledo, Toledo, Ohio*

ThP 367   **Probing the Mechanism of Zika Infection/Replication Using Lipidomics And Proteomics Analyses**; Roderick G. Davis; *Roskamp Institute, Sarasota, FL*

METABOLOMICS: CLINICAL APPLICATIONS
ThP 368-377

ThP 368   **Untargeted LC-MS/MS-based metabolic phenotyping applied to the CD248 knock out mouse model**; Neil J Loftus[1]; Emily Armitage[1]; Alan Barnes[1]; Janak Bechar[2]; Ed Rainger[3]; Matthew Harrison[3]; Ian D Wilson[4]; Christopher D Buckley[2]; Amy J Naylor[2]; *[1]Shimadzu MS/BU, Manchester, United Kingdom; [2]Rheumatology Research Group, Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; [3]Institute of Cardiovascular Sciences, University of Birmingham, Birmingham, United Kingdom; [4]Dept Metabolism, Digestion and Reproduction, Imperial College, London, United Kingdom*

ThP 369   **Clinical Validation of a LCMS Method for the Detection and Quantification of Salivary Dopamine, Epinephrine, and Serotonin**; Abu Hena Mostafa Kamal[1]; Kevin Zhu[1]; Lina Abi Mosleh[1]; Madison Roberts[1]; Gul Nowshad[1]; Mohamad Ammar Ayass[1]; *[1]Ayass BioScience, LLC, Frisco, TX*

ThP 370   **Metabolomics and lipidomics study of plasma from ischemic stroke patients for differentiation of subtypes of ischemic stroke**; Jianying Wang[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hung Hom, Hong Kong*

ThP 371   **Cigarette smoke alters fatty acid metabolism and promotes tumor progression in smokers diagnosed with bladder cancer**; Chandra S Amara[1]; Danthasinghe Waduge Badrajee Piyarathna[1]; Roni J. Bollag[2]; Martha K. Terris[2]; Lotan Yair[3]; Arun Sreekumar[1]; Shyam M. Kavuri[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Augusta Universuty, Augusta, GA; [3]UTSW, Dallas*

ThP 372   **Quantification of membrane lipids as biomarkers of aging relevant to Alzheimer's disease**; Gabriela Dovrtelova[1]; Petr Telensky[2]; Lukas Opalka[3]; Jana Klanova[4]; Aleš Hampl[4]; Jiri Damborsky[4]; Zdenek Spacil[4]; *[1]Masaryk University, Brno, Czech Republic; [2]Charles University, Prague, Czech Republic; [3]Charles University, Hradec Kralove, Czech Republic; [4]Masaryk University, Brno, Czech Republic*

ThP 373   **MRM-Based Measurement of CYP-Activity in relation to Dietary Modulators for Application to Cancer-Patient Serum and Dried Blood Samples**; Vincent R. Richard[1]; Constance A. Sobsey[1]; Noor Mady[2]; René P. Zahedi[1]; Robert Thomas Jagoe[2, 3]; Christoph H. Borchers[1, 3, 4]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [2]Peter Brojde Lung Cancer Centre, Jewish General Hospital, McGill Univertsity, Montreal, QC; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [4]Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

ThP 374   **Evaluation of lipidomic profiles of heart tissue in assessing the prognosis of patients undergoing advanced heart failure therapies**; Ashish Vaswani[1, 2]; Dr. Armando Alcazar Magana[1, 2]; Dr. Eric Zimmermann[3]; Dr. Jaishankar Raman[3, 4, 5]; Dr. Claudia Susanne Maier[1, 2]; *[1]Oregon State University, Corvallis, OR; [2]Department of Chemistry, Oregon State University, Corvallis, OR; [3]Oregon Health & Science University, Portland, Oregon; [4]St Vincent's Hospitals, Melbourne University, Melbourne, Australia; [5]Deakin University, Geelong & Melbourne, Melbourne, Australia*

ThP 375   **Metabolomics in precision medicine – are common software utilities and databases ready for its application?**; Stephen Barnes[1]; Ceren Yarar[1]; Jia Li[1]; Landon S Wilson[1]; Taylor F Berryhill[1]; Rebecca Howell[1]; Amie Mclain[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

ThP 377   **Metabolomic analysis of HIV-Associated Neuropathogenesis And Prodromal Alzheimer's Disease**; Emmanuel Elijah[1]; Nikesh Kumar[2]; Thomas Vollbrecht[3]; Alan K. Jarmusch[4]; Fernando Vargas[4]; Scott Letendre[3]; Kathleen Fisch[3]; Douglas Galasko[5]; Robert K Heaton[6]; Pieter C. Dorrestein[4]; Michelli Oliveira[3]; *[1]Dorrestein Lab-Skaggs School of Pharmacy and Pharmeceutical Sciences, La Jolla, CA; [2]Department of Medicine, University of California San Diego, La Jolla, CA; [3]Department of Medicine, University of California San Diego, La Jolla, 92093; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [5]Department of Neurosciences, University of California San Diego, La Jolla, CA; [6]Department of Psychiatry, University of California San Diego, La Jolla, CA*

METABOLOMICS: UNTARGETED METABOLITE PROFILING II
ThP 378-397

ThP 378   **Multi-omic characterisation of the mode of action of a potent new antimalarial compound, JPC-3210, against Plasmodium falciparum**; Geoff W Birrell[1]; Matthew P Challis[2]; Amanda De Paoli[2]; Dovile Anderson[2]; Shane M Devine[2]; Gavin D Heffernan[3]; David P Jacobus[3]; Michael D Edstein[1]; Ghizal Siddiqui[2]; Darren J Creek[2]; *[1]Australian Defence Force Malaria and Infectious Disease Institute, Brisbane, Australia; [2]Monash University, Melbourne, Australia; [3]Jacobus Pharmaceutical Company, Plainsboro, NJ*

ThP 379   **HPLC-HRMS global metabolomics approach for the diagnosis of Olive Quick Decline Syndrome markers in olive trees leaves**; Michael Zorzi[1]; Federica Dal Bello[1]; Riccardo Aigotti[1]; Alberto Asteggiano[1]; Claudio Medana[1]; *[1]University of Turin, Department of Molecular Biotechnology and Health Sciences, Torino, Italy*

ThP 380   **Untargeted Spatial Lipidomics of Colon Carcinoma Spheroids**; Fernando Tobias[1]; Amanda B. Hummon[1]; *[1]The Ohio State University, Columbus, OH*

ThP 381 **Exploring Bacterial Metabolome Alterations Mediated by Genetic Mutations**; Eric D Tague[1]; Sven Hackbusch[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

ThP 382 **Sphingolipid variations between hypertensive and normotensive patients elucidated by Magnetic Resonance Mass Spectrometry**; Eduardo Sommella[1]; Fabrizio Merciai[1]; Matthias Witt[2]; Jochen Friedrich[2]; Paola Di Pietro[1]; Pietro Campiglia[1]; [1]*University of Salerno, Fisciano, Italy;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

ThP 383 **4-dimensional annotation of Metabolomics features: CCS values as an additional source for higher confidence**; Ulrike Schweiger-Hufnagel[1]; Matthias Szesny[1]; Aiko Barsch[1]; Melvin Gay[2]; Torben Kimhofer[3]; Joel Gummer[3]; Luke Whiley[3]; Jeremy Nicholson[3]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Bruker Pty. LTD., Australia, Preston, Australia;* [3]*Murdoch University, Perth, Australia*

ThP 384 **Non-targeted fecal metabolomics in California mice to investigate the effect of early Genistein exposure on the gut microbiota-brain axis**; Saurav J Sarma[1, 2]; Brittney L Marshall[2, 3]; Yang Liu[2, 4]; Michelle J Farrington[2, 3]; Jiude Mao[2, 3]; Nathan J Bivens[2, 5]; Zhentian Lei[1, 2, 6]; Lloyd W Sumner[1, 2, 6]; Trupti Joshi[2, 4, 7]; Cheryl S Rosenfeld[2, 3, 4, 8, 9]; [1]*Metabolomics Center, University of Missouri, Columbia, MO;* [2]*Bond Life Sciences Center, University of Missouri, Columbia, MO;* [3]*Biomedical Sciences, University of Missouri, Columbia, MO;* [4]*MU Data Science and Informatics Institute, Columbia, MO;* [5]*DNA Core Facility, University of Missouri, Columbia, MO;* [6]*Department of Biochemistry, University of Missouri, Columbia, MO;* [7]*Department of Health Management and Informatics, University of Missouri, Columbia, MO;* [8]*Thompson Center for Autism and Neurobehavioral Disorders, University of Missouri, Columbia, MO;* [9]*Genetic Area Program, University of Missouri, Columbia, MO*

ThP 385 **Metabolite Profiling of Experimental Cutaneous Leishmaniasis Lesions Demonstrates Significant Perturbations in Tissue Phospholipids**; Adwaita R. Parab[1]; Diane Thomas[2]; Sharon Lostracco-Johnson[2]; Jair L Siqueira-Neto[2]; James Mckerrow[2]; Pieter C. Dorrestein[2, 3, 4]; Laura-Isobel Mccall[1]; [1]*Department of Microbiology and Plant Biology, University of Oklahoma, Norman, OK;* [2]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA;* [3]*Center for Microbiome Innovation, University of California San Diego, La Jolla, California;* [4]*Collaborative Mass Spectrometry Innovation Center, University of California San Diego, La Jolla, CA*

ThP 387 **Metabolic alterations observed in plasma of mice fed high-fat diet**; Ioanna Ntai[1]; Amanda Souza[1]; Ralf Tautenhahn[1]; Andreas Huhmer[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

ThP 388 **Annotating and identifying credentialed features in the yeast metabolome**; Dhanalakshmi S. Anbukumar[1]; Michaela Schwaiger-Haber[1]; Miriam Sindelar[1]; Ethan Stancliffe[1]; Gary J. Patti[1, 2]; [1]*Department of Chemistry, Washington University in St. Louis, St. Louis, MO;* [2]*Department of Medicine, Washington University in St. Louis, St. Louis, MO*

ThP 389 **Global Metabolic Landscape of Fusobacterium spp in Colorectal Cancer Cells.**; Hamzah Hassnein Ahmed[1]; Iqbal Mahmud, Phd[1]; Sasanka Sekhar Chukkapalli, Phd[1]; Ann Progulske-Fox, Phd[1]; Satya Narayan, Phd[1]; Timothy J Garrett, Phd[1]; [1]*University of Florida, Gainesville, FL*

ThP 390 **Using micro-scale sampling techniques for MS analysis of both extracellular and intracellular metabolites in drug-resistant spheroids**; Zongkai Peng[1]; Mei Sun[1]; Zhibo Yang[1]; [1]*University of Oklahoma, Norman, OK*

ThP 391 **UNTARGET LIPIDOMICS REVEALS A LIPIDS BIOMARKER PANEL AND KEY METABOLITES FOR THE DETECTION OF COLON CANCER**; Patrícia Oliveira Carvalho[1]; Anna Maria Alves De Piloto Fernandes[2]; Márcia Cristina Fernandes Messias[2]; Gustavo Henrique Bueno Duarte[2]; Gabrielle Kristine Doratiotto De Santis[2]; Andréia de Melo Porcari[2]; Ana Valéria Colnaghi Simionato[3]; Carlos Augusto Real Martinez[2]; [1]*Universidade São Francisco, Bragança Paulista, Brazil;* [2]*Universidade São Francisco, Bragança Paulista, Brazil;* [3]*Universidade Estadual de Campinas, Campinas, Brazil*

ThP 392 **A pre-gradient heart-cut method for online LC/LC-HRMS analysis of the hydrophilic and hydrophobic fractions of complex biological samples**; Kristian Pirttilä[1]; Curt Pettersson[1]; Mikael Hedeland[1]; [1]*Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden*

ThP 393 **Cancer Metabolic Rewiring in Host-Microbiota Interface**; Iqbal Mahmud[1]; Timothy J Garrett[2]; [1]*University of Florida, Gainesville, FL;* [2]*University of Florida, Gainesville*

ThP 394 **MicroLC-MS/MS Untargeted Metabolomics Analysis of Common Food Products**; Tong Shen[1]; Jeremiah Wells[1]; Tong Xie[2]; Remco Van Soest[3]; Arpana Vaniya[1]; Jacob Folz[1]; Oliver Fiehn[1]; [1]*West Coast Metabolomics Center, UC Davis, Davis, CA;* [2]*Jiangsu Key Laboratory of Pediatric Respiratory Disease, Nanjing University of Chinese Medicine, Nanjing, China;* [3]*SCIEX, Redwood Shores, CA*

ThP 395 **MDM2 Copy Number Aberrations Alter Lipid Metabolism in Liposarcoma Tumors, Impacting Response to Atorvastatin Treatment**; Andrew Patt[1]; Bryce Demoret[1]; Andrew Patterson[2]; Philip Smith[2]; James Chen[1]; Ewy Mathe[1]; [1]*The Ohio State University, Columbus, OH;* [2]*The Pennsylvania State University, University Park, PA*

ThP 396 **Differential metabolic responses of Saccharomyces cerevisiae in response to oxidants.**; Prajita Pandey[1]; Amit C. Gujar[2]; Vladimir Shulaev[1]; [1]*University of North Texas, Denton, TX;* [2]*Thermo Fisher Scientific, Austin, Texas*

ThP 397   **Application of DART-9.4T FT ICR MS to discovery of geo-location origin markers in small brown planthopper (Laodelphax striatellus)**; <u>Jong Bok Seo</u>[1]; Eui-Gil Jung[1]; Bo Yoon Seo[2]; Gwan Selk Lee[2]; Jinnyoung Choi[3]; [1]*Korea Basic Science Institute, Seoul, South Korea;* [2]*Department of Plant Protection, National academy of Agricultural Science, Jeonju, South Korea;* [3]*Broker Daltonics, South Korea, Seongnam, South Korea*

PEPTIDES: SEQUENCE ANALYSIS
ThP 398-405

ThP 398   **Detection, Evaluation and Validation of single amino acid variants in a PANC-1 Cell Line**; <u>Zhijing Tan</u>[1]; Jianhui Zhu[2]; Paul M. Stemmer[3]; Liangliang Sun[4]; Zhichang Yang[4]; Matthew J. Gaffrey[5]; Kendall Schultz[5]; Anthony J. Cesnik[6]; Xinpei Yi[7]; Michael R. Shortreed[8]; Tujin Shi[5]; David M. Lubman[1]; [1]*University of Michiagan, Ann Arbor, MI;* [2]*University of Michigan, Ann Arbor;* [3]*Wayne State University, Detroit, MI;* [4]*Michigan State University, East Lansing, MI;* [5]*PNNL, Richland, WA;* [6]*Stanford University, Stanford, CA;* [7]*Baylor College of Medicine, Houston, TX;* [8]*University of Wisconsin, Madison, WI*

ThP 399   **Ex vivo degradation of bioactive peptides in equine plasma studied by HILIC-HRMS**; <u>Fuyu Guan</u>[1, 2]; Savannah Fay[1, 2]; Xiaoqing Li[1, 2]; Youwen You[1, 2]; Mary A Robinson[1, 2]; [1]*University of Pennsylvania, Kennett Square, PA;* [2]*PA Equine Toxicology and Research Laboratory, West Chester, PA*

ThP 400   **Analytical Artifacts and Mitigation Strategies for Sequence Variance Analysis by Peptide Mapping**; <u>Stone D.-H. Shi</u>[1]; Neelam Khanal[1]; Andrew Dykstra[1]; Christopher S Spahr[1]; Zhongqi Zhang[1]; [1]*Amgen, Thousand Oaks, CA*

ThP 401   **A General Strategy to Improve de Novo Peptide Sequencing based on Deep Learning**; <u>Shaokai Wang</u>[1]; Bin Ma[1]; [1]*University of Waterloo, Waterloo, ON*

ThP 402   **Force degraded product identification of Liraglutide drug by Mass Spectrometer**; <u>Shadab Ahmad</u>[1]; Sharwan Kumar[1]; Dipankar Malakar[1]; Manoj Pillai[1]; [1]*Sciex, Gurugram, India*

ThP 403   **Differentiating isomeric amino acid residues in peptides with charge transfer dissociation mass spectrometry (CTD-MS)**; <u>Halle M. Edwards</u>[1]; Praneeth M. Mendis[1]; Zachary J. Sasiene[1]; Hoi-Ting Wu[2]; Ryan R. Julian[2]; Glen P. Jackson[1, 3]; [1]*C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV;* [2]*Department of Chemistry, University of California, Riverside, Riverside, CA;* [3]*Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 404   **Identification of Therapeutic Peptides and of its Impurities**; Ashish Pargaonkar[1]; <u>Laxmi Reddy</u>[2]; Venkat Reddy[2]; Srinivasulu Polysetty[2]; Saurabh Nagpal[3]; Chidella Kartheek Srinivas[4]; Saikat Banerjee[5]; [1]*Agilent Technologies India Pvt Ltd, Bengaluru, India;* [2]*MSN Laboratories Pvt Ltd, Hyderabad, India;* [3]*Agilent Technologies India Pvt Ltd, Manesar, India;* [4]*Agilent Technologies, BENGALURU, India;* [5]*Agilent Technologies India Pvt Ltd, Hyderabad, India*

ThP 405   **Exploring the diversity of cysteine-rich natural product peptides via MS/MS fingerprint ions**; <u>Nicole C Parsley</u>[1]; Owen L. Williams[1]; Leslie M. Hicks[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

PEPTIDOMICS
ThP 406-425

ThP 406   **Native Peptidomics- An HPLC-MS/MS Approach for Analysis of Tumors' Signature**; Stefan Wolfsberger[1]; Tanja Panić-Janković[2]; Sonja Seyfert[2]; Umesh Kalathiya[3]; Javier Alfaro[3]; Ted Hupp[4]; <u>Goran Mitulovic</u>[2]; [1]*Department of Neurosurgery at the Medical University of Vienna, Vienna, Austria;* [2]*Medical University of Vienna, KIMCL, Vienna, Austria;* [3]*Uiversity of Gdansk, Gdansk, Poland;* [4]*University of Edinburgh, Edinburgh, United Kingdom*

ThP 408   **DIA MS for Profiling the Neuropeptidomic Changes in Cancer borealis Hemolymph Resulting from Food Intake**; <u>Wenxin Wu</u>[1]; Kellen DeLaney[1]; Lingjun Li[1]; [1]*University of Wisconsin-Madison, Madison, Wisconsin*

ThP 409   **Chromium(III)-Induced Enhanced Protonation Survey of Peptides in Electrospray Ionization**; <u>Nnenna E. Dieke</u>[1]; Carolyn J. Cassady[1]; [1]*The University of Alabama, Tuscaloosa, AL*

ThP 410   **Neuropeptidomic Study of the Mammalian Subcommissural Organ (SCO) by High Resolution Mass Spectrometry**; <u>Pingli Wei</u>[1]; Fengfei Ma[2]; Woo-Ping Ge[3, 4, 5, 6]; 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]*Children's Research Institute, University of Texas Southwestern Medical Center, Dallas, TX;* [4]*Department of Pediatrics, University of Texas Southwestern Medical Center, Dallas, TX;* [5]*Department of Neuroscience, University of Texas Southwestern Medical Center, Dallas, TX;* [6]*Department of Neurology and Neurotherapeutics, University of Texas Southwestern Medical Center, Dallas, TX*

ThP 411   **Label-free and DiLeu isobaric tag quantitative methods for profiling mouse hypothalamic neuropeptidomic and proteomic changes under different gut microbiota environments**; <u>Rui Liu</u>[1]; Pingli Wei[2]; Caitlin Keller[3]; Dustin Frost[3]; Shuying Han[1]; Tzu-Wen Cross[3]; Federico Rey[3]; Lingjun Li[3]; [1]*Nanjing University of Chinese Medicine, Nanjing, China;* [2]*University of Wisconsin-Madison, Madison, WI;* [3]*University of Wisconsin-Madison, Madison, Wisconsin*

ThP 412   **Development of an automated MHC-associated peptide enrichment method for immunopeptidomics analysis using AssayMAP large capacity cartridges**; Samuel Pollock[1]; Shuai Wu[2]; Jerry Han[2]; Steve Murphy[2]; *[1]Genentech, Inc., South San Francisco, CA; [2]Agilent Technologies, Santa Clara, CA*

ThP 413   **Development of Method for Quantitation and Localization of Hyperglycemic Hormones Implicated in Crustacean Response to Hypoxia**; Nhu Quynh Vu[1]; Dustin Frost[1]; Amanda Rae Buchberger[1]; Hsu-Ching Yen[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, Wisconsin*

ThP 414   **Profiling, imaging, and functional assessment of neuropeptides in the crustacean cardiac neuromuscular system using DIA-MS**; Kellen Delaney[1]; Tessa Hellenbrand[1]; Lingjun Li[1]; *[1]University of Wisconsin, Madison, Madison, WI*

ThP 415   **Profiling TOPs-mediated proteolytic pathways in Arabidopsis thaliana**; Anthony A. Iannetta[1]; Holden T. Rogers[1]; Thualfeqar Al-Mohanna[2]; George V. Popescu[2]; Sorina C. Popescu[2]; Leslie M. Hicks[1]; *[1]UNC Chapel Hill, Chapel Hill, NC; [2]Mississippi State University, Starkville, MS*

ThP 416   **CAatlas: an immunopeptidome atlas of human cancer**; Xinpei Yi[1, 2]; Yuxing Liao[1, 2]; Kai Li[1, 2]; Bo Wen[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*

ThP 417   **Characterisation of a putative new metabolic hormone in human plasma**; Michelle Cielesh[1]; Dylan J Harney[1]; Mark Larance[1]; *[1]Charles Perkins Centre, School of Life and Environmental Sciences, University of Sydney, Sydney, Australia*

ThP 418   **Enhanced identification of bioactive peptides in meat hydrolysates by 4D peptidomics**; Evelyne Maes[1]; Stephen Haines[1]; Michael Krawitzky[2]; Christopher Adams[2]; Gary Kruppa[2]; Ancy Thomas[1]; Stefan Clerens[1, 3, 4]; *[1]AgResearch, Christchurch, New Zealand; [2]Bruker Daltonics, San Jose, CA; [3]Biomolecular Interaction Centre (Canterbury University), Christchurch, New Zealand; [4]Riddet Institute (Massey University), Palmerston North, New Zealand*

ThP 419   **Identification and characterization of signaling Proteolytic Cleavage Products (PCPs) of proteins in the Plant-Microbe Interface**; Him K Shrestha[1, 2]; Ivan Villalobos Solis[1, 2]; Suresh Poudel[2]; Clemence Bonnot[3]; Claire Veneault-Fourrey[3]; Francis Martin[3]; Paul Abraham[2]; Robert Hettich[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; [3]UMR 1136 INRA-Université de Lorraine 'Interactions Arbres/Microorganismes', Laboratoire d'Excellence ARBRE, Centre INRA-Lorraine, Champenoux, France*

ThP 420   **Characterization of neuropeptide proteoforms in human cerebrospinal fluid**; Savannah E. Kandigian[1]; James P. Quinn[1]; Bianca A. Trombetta[1]; Steven E. Arnold[1]; Becky C. Carlyle[1]; *[1]Massachusetts General Hospital and Harvard Medical School, Charlestown, MA*

ThP 421   **Increasing the coverage of the immunopeptidome by combining mild acid elution and immunoprecipitation analyzed by trapped ion mobility spectrometry(tims)-TOF**; Teesha C. Luehr[1, 2]; Morris Young[1, 2]; Leonard J. Foster[1, 2]; *[1]Michael Smith Laboratories, Vancouver, BC; [2]University of British Columbia, Vancouver, BC*

ThP 422   **Immuno-peptidomics: Utilizing cloud computing to identify more peptides in a fraction of the search time**; Amol Prakash[1]; Benjamin Orsburn[2]; *[1]Optys Tech Corporation, Shrewsbury, MA; [2]Proteomic Und Genomic Sciences, Columbia, 21406*

ThP 423   **An Improved Peptidomics Workflow Using a Multi-nozzle Electrospray Emitter for Capillary Flows**; Bertrand Rochat[1, 2]; Jachen Barblan[1, 2]; Patrice Waridel[1, 2]; Manfredo Quadroni[1, 2]; *[1]University of Lausanne, Lausanne, Switzerland; [2]Protein Analysis Facility, Lausanne, Switzerland*

ThP 424   **Discovery of Tumor associated T cell epitopes through targeted searches of mass spectrometry data**; Prathyusha Konda[1]; Patrick Murphy[2]; Shashi Gujar[1]; *[1]Dalhousie University, Halifax, NS; [2]PEI University, Prince Edward Island, PEI*

ThP 425   **An evaluation of spectral assignments in two spliced peptide studies reveals errors leading to false positive assignments**; Cheryl F. Lichti; *Department of Pathology & Immunology and The Bursky Center for Human Immunology and Immunotherapy Programs, Washington University, St. Louis, MO*

PHOSPHOPEPTIDES: ENRICHMENT METHODS
ThP 426-430

ThP 426   **Zirconium(IV)-IMAC for phosphopeptide enrichment in mass spectrometry driven phosphoproteomics**;
Ignacio Arribas Díez[1]; Ireshyn Govender[2]; Previn Naicker[2]; Stoyan Stoychev[2, 3]; Justin Jordaan[2, 3]; Ole N Jensen[1];
*[1]University of Southern Denmark, Odense, Denmark; [2]Council for scientific and industrial research, Pretoria, South
Africa; [3]ReSyn BioSciences, Pretoria, South Africa*

ThP 427   **Exploring the dual-functional characteristics of Ti(IV)-IMAC and its application in glycopeptide,
phosphopeptide and M6P glycopeptide enrichment and separation**; Junfeng Huang[1]; Xiaoyan Liu[2]; Danqing
Wang[1]; Yusi Cui[1]; Xudong Shi[1]; Jing Dong[2]; Mingliang Ye[2]; Lingjun Li[1]; *[1]University of Wisconsin-Madison,
Madison, WI; [2]Key Laboratory of Separation Sciences for Analytical Chemistry, National Chromatographic R&A
Center, Dalian In-stitute of Chemical Physics, Chinese Academy of Sciences (CAS), Dalian, China*

ThP 428   **The application of DNA aptamer in phosphoproteomics**; Hsuan-Kuang Liu; *National Taiwan Ocean University,
Keelung City, Taiwan*

ThP 429   **Efficiency of INtip extractions for peptide desalting and phosphopeptide enrichments using commercially
available automated liquid handling systems**; Brian T Mullis[1]; Lim Andrew Lee[2]; Rebekah Woolsey[3]; David
Quilici[3]; Qian Wang[1]; *[1]University of South Carolina, Columbia, SC; [2]Integrated Micro-Chromatography Systems,
Irmo, SC; [3]Mitch Hitchcock, Ph.D. Nevada Proteomics Center, Reno, NV*

ThP 430   **Global phosphoproteomic analysis from low sample amounts enabled by effective phosphopeptide
enrichment**; Fang Liu[1]; Momei Zhou[2]; Kratika Singhal[1]; Rowan Matney[1]; Stefan L. Oliver[2]; Ann M. Arvin[2]; Ryan D.
Leib[1]; Allis S. Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford University, Stanford, CA; [2]Departments of
Pediatrics and Microbiology & Immunology, Stanford University School of Medicine, Stanford, CA*

PLANTS: SYSTEMS, BIOTECHNOLOGY, AND NATURAL PRODUCTS
ThP 431-441

ThP 431   **An international laboratory comparison of dissolved organic matter composition by high resolution mass
spectrometry: Are we getting the same answer?**; Jeffrey A. Hawkes[1]; Juliana D'andrilli[2]; Rachel L. Sleighter[3];
Hongmei Chen[3]; Patrick G. Hatcher[3]; Amna Ijaz[4]; Maryam Khaksari[4]; Simeon Schum[4]; Lynn Mazzoleni[4]; Rosalie
K. Chu[5]; Nikola Tolic[5]; William Kew[5]; Nancy Hess[5]; Jitao Lv[6]; Shuzhen Zhang[6]; Chen He[7]; Quan Shi[7]; Ryan H. S.
Hutchins[8]; Diana C. Palacio Lozano[9]; Remy Gavard[9]; Hugh E. Jones[9]; Mary J. Thomas[9]; Mark P. Barrow[9]; Helena
Osterholz[10]; Thorsten Dittmar[10]; Carsten Simon[11]; Gerd Gleixner[11]; Stephanie M. Berg[12]; Christina K. Remucal[12];
Núria Catalán[13]; Richard B. Cole[14]; Beatriz E. Noriega-Ortega[15]; Gabriel Singer[15]; Nikola Radoman[16]; Nicholas D.
Schmitt[17]; Aron Stubbins[17]; Jeffrey N. Agar[17]; Phoebe Zito[18]; David C. Podgorski[18]; *[1]Uppsala University, Uppsala,
Sweden; [2]Louisiana Universities Marine Consortium, Chauvin, LA; [3]Old Dominion University, Norfolk, VA;
[4]Michigan Technological University, Houghton, MI; [5]PNNL, Richland, WA; [6]Chinese Academy of Sciences, Beijing,
China; [7]China University of Petroleum, Beijing, China; [8]University of Alberta, Edmonton, AB; [9]University of
Warwick, Coventry, United Kingdom; [10]Carl von Ossietzky University, Oldenburg, Germany; [11]Max Planck Institute,
Jena, Germany; [12]University of Wisconsin, Madison, WI; [13]Catalan Institute for Water Research, Girona, Spain;
[14]Sorbonne Université, Paris, France; [15]Leibniz Institute of Freshwater Ecology and Inland Fisheries, Berlin,
Germany; [16]Stockhom University, Stockholm, Sweden; [17]Northeastern University, Boston, MA; [18]University of New
Orleans, New Orleans, LA*

ThP 432   **A large GSK3 signaling network is uncovered by a combination of proximity labeling and
phosphoproteomics in Arabidopsis**; Chuan-Chih Hsu[1]; Chao Ho Park[1]; Tae-Wuk Kim[2]; Jia-Ying Zhu[1]; Yu-Chun
Hsiao[1]; Shou-Ling Xu[1]; Zhi-Yong Wang[1]; *[1]Carnegie Institution for Science, Stanford, CA; [2]Hanyang University,
Seoul, South Korea*

ThP 433   **Preserved and variable spatial-chemical changes of lipids across leaves in response to wounding**; Dusan
Velickovic[1]; Rosalie K. Chu[1]; Corinna Henkel[2]; Annika Koch[2]; Nannan Tao[3]; Joshua N Adkins[1]; Christopher
Anderton[1]; Jennifer E. Kyle[1]; Kent Bloodsworth[1]; Lisa M Bramer[1]; Shannon Cornett[4]; Kristin E. Burnum-Johnson[1];
*[1]PNNL, Richland, WA; [2]Bruker, Bremen, Germany; [3]Bruker Scientific, San Jose, CA; [4]Bruker Scientific LLC,
Billerica, MA*

ThP 434   **Defining Core Leaf and Root Metabolomes for Sorghum Grown in the Midwestern United States**; Amy
Sheflin[1]; Daniel P. Schachtman[2]; Ellen L. Marsh[2]; Peng Liu[3]; Hao Wang[3]; Corey D Broeckling[1]; Jessica E Prenni[1];
*[1]Colorado State University, Fort Collins, CO; [2]University of Nebraska-Lincoln, Lincoln, NE; [3]Iowa State University,
Ames, IA*

ThP 435   **Quantitative proteomics reveals details of the susceptibility pathway of Septoria canker mediated by a
Populus trichocarpa G-type lectin receptor-kinase**; Ryan R. Lenz[1, 2]; Paul E. Abraham[3]; Jessy Labbe[3];
Wellington Muchero[3]; Robert L. Hettich[3]; Jared M. Leboldus[1]; *[1]Oregon State University, Corvallis, OR; [2]DOE Office
of Science Graduate Student Research (SCGSR), Oak Ridge, TN; [3]Oak Ridge National Laboratory (ORNL), Oak
Ridge, TN*

ThP 436   **Top-down proteomics in plant biology: large-scale delineation of proteoforms in Arabidopsis leaf tissue**;
Qianjie Wang; *Michigan State University, East Lansing, MI*

ThP 437   **Proteomic analysis of Chelidonium majus plant latex upon potyvirus inoculation using 2-D electrophoresis and tandem mass spectrometry**; Michalina Krakowiak[1]; Sophia Bałdysz[1]; Oskar Musidlak[1]; Robert Nawrot[1]; [1]*Adam Mickiewicz University in Poznan, Faculty of Biology, Laboratory of Molecular Virology, Poznan, Poland*

ThP 438   **Diterpene metabolism study in Jatropha curcas L using targeted proteomics methods**; Natália P. Almeida[1]; Domingos F. Neto[2]; Gabriel R. A. Carneiro[3]; Andreza R. B. Farias[2]; Gilberto B. Domont[1]; Francisco A. P. Campos[4]; Fabio CS Nogueira[1, 3]; [1]*Proteomics Unit, Institute of Chemistry, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, Rio de Janeiro, Brazil; [2]Department of Agricultural Sciences, Federal University of Ceará, Fortaleza, Brazil; [3]Laboratory of Proteomics/LADETEC, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [4]Department of Biochemistry and Molecular Biology, Federal University of Ceará, Fortaleza, Brazil*

ThP 439   **Time-based metabolomics profiling of innate immunity and infection response in fungal-resistant rice**; Joshua Blakeslee[1]; Rachel Combs[1]; Pengfei Bai[2]; Matthew Bernier[2]; Nick Choi; Guo-Liang Wang[2]; [1]*The Ohio State University, Wooster, OH; [2]The Ohio State University, Columbus, OH*

ThP 440   **Enhanced characterization of lignin oligomers and phenolic compounds using CID-MSn combined with HCD-MS2**; Woo-Young Song[1]; Tae-Young Kim[1]; [1]*Gwangju Institute of Science and Technology, Gwangju, South Korea*

ThP 441   **The tomato root exometabolome and iron-limitation induced changes in exudation profiles**; Vineeta Rai[1]; Oliver Baars[1]; [1]*North Carolina State University, Raleigh, NC*

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ThP 442   **Laser Processing of Fiber Biopolymers by using Infrared Free Electron Laser Combined with ESI-MS Analysis**; Takayasu Kawasaki[1]; Takeshi Sakai[2]; Yoske Sumitomo[2]; Ken Hayakawa[2]; Kyoko Nogami[2]; Heishun Zen[3]; Akinori Irizawa[4]; Yasushi Hayakawa[2]; [1]*IR Free Electron Laser Research Center, Tokyo University of Science, Noda, Japan; [2]Laboratory for Electron Beam Research and Application (LEBRA), Nihon University, Funabashi, Japan; [3]Institute of Advanced Energy, Kyoto University, Uji, Japan; [4]The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Japan*

ThP 443   **Optimisation of Polymer Photoligation Reactions Using Laser Photodissociation Action Spectroscopy**; David L. Marshall[1]; Jan Philipp Menzel[2]; Benjamin I. Mckinnon[3]; Adam J. Trevitt[3]; Christopher Barner-Kowollik[1]; Stephen J. Blanksby[1]; [1]*Queensland University of Technology, Brisbane, Australia; [2]Queensland University of Technology, Brisbane, Australia; [3]University of Wollongong, Wollongong, Australia*

ThP 444   **Ultraviolet irradiation degradation analysis of polyethylene terephthalate film using matrix assisted laser desorption/ionization mass spectrometry imaging**; Takaya Satoh[1]; Yusuke Sakuda[1]; Sayaka Nakamura[2]; Thierry Fouquet[2]; Hiroaki Satoh[2]; Yoshihisa Ueda[1]; Glen Gregory[3]; [1]*JEOL Ltd, Akishima, Japan; [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [3]JEOL USA, Inc., Peabody, MA*

ThP 445   **Differentiation of Macrocyclic and Tadpole Isomers Using UPLC-MS/MS and Radical-Induced Fragmentation Chemistry**; Jason M O'neill[1]; Scott M Grayson[2]; Chrys Wesdemiotis[1]; [1]*The University of Akron, Akron, OH; [2]Tulane University, New Orleans, Louisiana*

ThP 446   **Rapid fingerprinting of high-molecular-weight polymers containing C-O, Si-O or C-S bonds by Desorption Ionization Using Through-Hole Alumina Membranes (DIUTHAME)**; Sayaka Nakamura[1]; Thierry Nicolas Jean Fouquet[1]; Robert B. Cody[2]; Takayuki Ohmura[3]; Masahiro Kotani[3]; Hiroaki Sato[1]; Yasuhide Naito[4]; [1]*National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; [2]JEOL USA, Inc., Peabody, MA; [3]Hamamatsu Photonics K.K., Iwata, Japan; [4]The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan*

ThP 447   **Analysis of Polymer Additives in Plastic Food Containers Using the Quadrupole TOF Mass Spectrometer**; Takahiro Goda[1]; Junichi Masuda[1]; Manami Kobayashi[1]; Yoshihiro Hayakawa[2]; [1]*Shimadzu Corporation, Hadano, Japan; [2]Shimadzu corporation, Kyoto, Japan*

ThP 448   **Multiplexed Mass Spectrometric Screening of the Cellular Uptake of Polymer Based Drug Delivery Vehicles Using MALDI-MS**; Dheeraj K. Agrohia; *University of Massachusetts, Amherst, AMHERST, MA*

ThP 449   **Ultraviolet Photo-activation using Synchrotron Radiation for Tandem Mass Spectrometry of Polysiloxanes**; Inès Aloui[1]; Véronique Legros[1]; Alexandre Giuliani[2]; William Buchmann[1]; [1]*Université Paris-Saclay, Univ Evry, CNRS, LAMBE, Evry, France; [2]Disco Beamline, Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Gif-sur-Yvette, France*

ThP 450   **Characterization of fuel cell ionomer membrane degradation by LC-MS**; Kyle Kalstabakken[1]; Michael Yandrasits[1]; Matthew Lindell[1]; Eric Fort[2]; [1]*3M, St. Paul, MN; [2]University of St. Thomas, St. Paul, MN*

ThP 451   **Characterizing photoresist films at the nanoscale with mass spectrometry**; Michael Eller[1]; Mingqi Li[2]; Xisen Hou[2]; Stanislav Verkhoturov[3]; Emile Schweikert[3]; Peter Trefonas[2]; [1]*California State University Northridge, Northridge, CA; [2]DuPont Electronics and Imaging, Marlborough, MA; [3]Texas A&M University, College Station, TX*

ThP 452 **Ion-mobility separation behavior of synthetic polymer samples affected by adduct cation**; Toshiji Kudo[1]; Yoshifumi Mori[1]; Takashi Nirasawa[1]; Shigeru Sakamoto[1]; Christopher Thompson[2]; [1]*Bruker Japan, Yokohama, Japan;* [2]*Bruker Scientific LLC, Billerica, MA*

ThP 453 **PolymerSoup: A Novel Tool for De Novo Sequencing of Polymer Mixtures**; David Doran[1]; Emma Clarke[1]; Graham Keenan[1]; Emma J Carrick[1]; Cole Mathis[1]; Leroy Cronin[1]; [1]*University of Glasgow, Glasgow, United Kingdom*

ThP 454 **IDENTIFICATION OF UNKNOWN ADDITIVES IN POLYETHYLENE BY SINGLE QUADROPOLE LC-MS**; Peter Shimeall[1]; L. Shayne Green[1]; [1]*Dow Chemical, Lake Jackson, TX*

ThP 455 **Interpreting a complex ion mobility-mass spectrometry analysis of a modified statistical copolymer**; Jean R. N. Haler[1]; Jessica Desport[1]; Edwin De Pauw[2]; Luc Patiny[3]; Gilles Frache[1]; [1]*Luxembourg Institute of Science and Technology, Belvaux, Luxembourg;* [2]*University of Liege, Liège, Belgium;* [3]*Zakodium Sàrl, -, Switzerland*

ThP 456 **Agnostic Polymer Detection Using Mass Spectrometry for Astrobiological Samples**; Victoria Da Poian[1]; Luoth Chou[1]; Natalie Grefenstette[2]; Heather Graham[1]; Chris Kempes[2]; Paul Mahaffy[1]; Sarah Stewart Johnson[1]; [1]*NASA Goddard Space Flight Center, Greenbelt, MD;* [2]*Santa Fe Institute, Santa Fe, NM*

PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION
ThP 457-483

ThP 457 **Characterization of Low Molecular Weight (LMW) Impurities using Intact HILIC-MS**; Daniel Michael Waldera-Lupa[1]; Heiner Falkenberg[1]; Sylvia Aretz-Meyer[1]; Anna Lendzian[1]; Ronja Schwichtenhövel[1]; Eva Ennemann[1]; Marcus Mreyen[1]; Roland Moussa[1]; [1]*Protagen Protein Services, Dortmund, Germany*

ThP 458 **Use of PASEF for Accelerated Protein Sequence Confirmation and de novo Sequencing with High Data Quality**; Stuart Pengelley[1]; Waltraud Evers[1]; Eckhard Belau[1]; Ilker Sen[2]; Wilfred Tang[2]; Alain Beck[3]; Detlev Suckau[1]; [1]*Bruker Daltonics, Bremen, Germany;* [2]*Protein Metrics Inc., Cupertino, CA;* [3]*IRPF, Centre d'Immunologie Pierre Fabre, St-Julien en Genevois, France*

ThP 459 **A deconvolution algorithm for efficient discrimination between real and artefactual, harmonic signals in intact mass analysis of a bispecific antibody**; Peter Haberl[1]; Jonathan Jones[2]; Catherine Evans[3]; Maurizio Bronzetti[4]; [1]*Genedata GmbH, Munich, Germany;* [2]*Genedata Ltd, Cambridge, United Kingdom;* [3]*Genedata AG, Basel, Switzerland;* [4]*Genedata Inc, San Francisco, CA*

ThP 460 **Intact Protein Multi-Attribute Method (MAM) that Includes the Identification and Quantification of Protein Clipping Events**; Lars Vorwerg[1]; Stuart Pengelley[1]; Waltraud Evers[1]; Eckhard Belau[1]; Detlev Suckau[1]; [1]*Bruker Daltonics, Bremen, Germany*

ThP 461 **Rapid and Confident Identification of Expected and Scrambled Disulfide Bonds in Biologics**; Severine Clavier[1]; Hélène Le Borgne[1]; Bruno Genet[1]; Sean Mc Carthy[2]; Kerstin Pohl[2]; [1]*Sanofi, Vitry Sur Seine, France;* [2]*Sciex, Framingham, MA*

ThP 462 **Enhancing the characterization of adeno-associated virus (AAV) vectors by improved UPLC and MS methodology**; Ximo Zhang[1]; Stephan Koza[2]; Hua Yang[1]; Lindsey Organtini[1]; Henry Shion[1]; Kamran Anwar[3]; Daniel Gailbraith[3]; Ying Qing Yu[2]; Weibin Chen[2]; [1]*Waters Corporation, Milford, MA;* [2]*Waters Corps, Milford, MA;* [3]*BioReliance, Rockville, MD*

ThP 463 **An automated MS data processing workflow for sensitive detection of low-abundance sequence variants in biopharmaceuticals**; Aude Tartiere[1]; Jonathan Jones[2]; Catherine Evans[3]; Peter Haberl[4]; Maurizio Bronzetti[1]; [1]*Genedata Inc, San Francisco, CA;* [2]*Genedata Ltd, Cambridge, United Kingdom;* [3]*Genedata AG, Basel, Switzerland;* [4]*Genedata GmbH, Munich, Germany*

ThP 464 **Characterization of Disulfide Bonds in Bevacizumab Biosimilar Using A Q-TOF Mass Spectrometer**; Yonghai Lu[1]; Jie Xing[2]; Zhaoqi Zhan[2]; [1]*Shimadzu (Asia Pacific) PTE LTD, Singapore, Singapore;* [2]*Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore*

ThP 465 **Monoclonal antibody characterization through native Orbitrap mass spectrometry leading to improved sensitivity and microheterogeneity elucidation**; Sara Carillo[1]; Florian Fussl[1]; Itzcoatl Gomez Aquino[2]; Ioscani Jimenez Del Val[2]; Jonathan Bones[1, 2]; Silvia Millan Martin[1]; [1]*National Institute for Bioprocessing Research and Training (NIBRT), blackrock, Ireland;* [2]*University College of Dublin, Dublin, Ireland*

ThP 466 **Purity and Identity Characterization of Adeno-Associated Virus Capsid Particles by Intact and Bottom-Up Based Liquid Chromatography-Mass Spectrometry Methods**; Wendi Hale[1]; Dominique Garceau[2]; Tristan Cano[2]; Caitlin Jaeger[2]; Roy Hegedus[2]; William Hermans[2]; Norman Garceau[2]; Christopher M. Colangelo[1]; [1]*Agilent, Lexington, MA;* [2]*LakePharma, Worcester, MA*

ThP 467 **Intact Mass Analysis using Automated Time-resolved Deconvolution: In-depth Characterization of IgG-type Monoclonal Antibody Subunits**; Kate Liu[1]; David Bush[2]; Jonathan Jones[3]; Catherine Evans[4]; Maurizio Bronzetti[1]; [1]*Genedata Inc, San Francisco, CA;* [2]*Genedata, Lexington, MA;* [3]*Genedata Ltd, Cambridge, United Kingdom;* [4]*Genedata AG, Basel, Switzerland*

ThP 468   **Improving the analysis of adeno-associated virus (AAV) capsid proteins by a LC-FLR/MS approach for AAV-based gene therapy development**; Xiaoying Jin[1]; Ximo Zhang[2]; Zichuan Zhang[1]; Lin Liu[1]; Qiyu Wang[1]; Yunfan Gao[1]; Joanne Cotton[1]; Stephan Koza[2]; Ying Qing Yu[2]; Weibin Chen[2]; Marc Verhagen[1]; Karen Lee[1]; Claire Davies[1]; *[1]Sanofi, Framingham, MA; [2]Waters Corporation, Milford, MA*

ThP 469   **Biotherapeutic Characterization in Fifteen Minutes: Structures for Lossless Ion Manipulations (SLIM) Ion Mobility for Critical Quality Attribute Identification and Monitoring**; James R. Arndt[1]; Kelly L. Wormwood Moser[1]; Liulin Deng[1]; Anisha Yadav[1]; Stephen Krufka[1]; Daniel Debord[1]; Laura Maxon[1]; *[1]Mobilion Systems, Inc., Chadds Ford, PA*

ThP 470   **Identification and Quantitative Analysis of Disulfide Scrambling Events for In-Depth Characterization Studies of Therapeutic Proteins**; Magdalena Widgren Sandberg[1]; Jakob Bunkenborg[1]; Thomas Kofoed[1]; Kerstin Pohl[2]; *[1]Alphalyse A/S, Odense, Denmark; [2]Sciex, Framingham, MA*

ThP 472   **Impact of media components (Vitamins) supplementation on glycan profile as a critical quality attribute of an in-house produced monoclonal Antibody**; Rohan Shah[1]; Saurabh Nagpal[2]; Anurag S Rathore[1]; *[1]Department of Chemical Engineering, Indian Institute of Technology, Delhi, India; [2]Agilent technologies, Gurgaon, India*

ThP 473   **Glycosylation Profiling of Rituximab using HILIC-LC-FLD glycan mapping and RP-LC-MS glycopeptide mapping**; Hongbin Zhu[1]; Joshua Shipman[2]; Milani Rasangika Wijeweera Patabandige[3]; Jason Rodriguez[1]; Connie Ruzicka[1]; David Keire[1]; *[1]U.S. FDA, Saint Louis, MO; [2]FDA, Saint Louis, MO; [3]University of Kansas, Lawrence, KS*

ThP 474   **Characterization and Differentiation of Bispecific Monoclonal Antibodies by Native Mass Spectrometry**; Chen Du[1, 2]; Zachary L VanAernum[1, 2]; Wilson Phung[3]; Guanghui Han[4]; Wendy Sandoval[3]; Vicki H Wysocki[1, 2]; *[1]The 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 Microchemistry, Proteomics and Lipidomics, Genentech, Inc., South San Francisco, CA; [4]San Jose Mass Spectrometry Center, BGI Americas, San Jose, CA*

ThP 475   **Characterization of Heavily Glycosylated Therapeutics via Proton Transfer Charge Reduction (PTCR)**; Fred Zinnel[1]; Hirsh Nanda[2]; Harsha Gunawardena[2]; *[1]Thermo Fisher Scientific, Somerset, NJ; [2]JOHNSON AND JOHNSON, Spring House, PA*

ThP 477   **Understanding the structural basis for Alpha-Synuclein aggregation by Fast Photochemical Oxidation of Proteins**; Ravi Kant[1]; Prashant N. Jethva[2]; Saketh Chemuru[1]; Harish Kumar[3]; Eva Illes-Toth[2]; Jing Yan[1]; Michael L. Gross[1]; *[1]Washington University, St Louis, MO; [2]Washington University, St. Louis, MO; [3]National Centre for Biological Sciences, Bangalore, India*

ThP 478   **Fighting Counterfeits for Biopharmaceuticals with Accurate Mass Spectrometry**; Kerstin Pohl[1]; Esme Candish[2]; Sean Mccarthy[2]; *[1]SCIEX, Framingham, MA; [2]Sciex, Framingham, MA*

ThP 479   **Coupling a Microchip-Based Imaged cIEF Separation via ESI to Multiple Mass Spectrometry Platforms for Intact Antibody Characterization**; Mariam S Elnaggar[1]; Christopher Herring[1]; Scott Mack[1]; Maggie A. Ostrowski[1]; Erik Gentalen[1]; *[1]Intabio, Inc., Newark, CA*

ThP 480   **Characterization of Charge Heterogeneity of Monoclonal Antibodies Using Microchip CE coupled with TOF MS**; Zuzana Demianova[1]; Fang Wang[1]; Sean Mccarthy[2]; J. Scott Mellors[3]; Joshua Guerrette[3]; Kerstin Pohl[2]; *[1]Sciex, Brea, CA; [2]Sciex, Framingham, MA; [3]908 Devices, Inc., Boston, MA*

ThP 481   **Integrating proton transfer charge reduction, multiple ion activations and synchronous precursor selection improves middle-down analysis of antibodies and antibody-drug conjugates**; Ryan Oates[1]; Kristina Srzentic[2]; Christopher Mullen[3]; Romain Huguet[3]; Vlad Zabrouskov[3]; John E.P. Syka[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Fisher Scientific, Cambridge Proteomics Research Group, Cambridge, MA; [3]ThermoFisher Scientific, San Jose, CA*

ThP 482   **Monitoring Local High Order Structure Change for Stressed Biotherapeutics using Native Digestion Peptide Mapping**; Dongdong Wang; *BioAnalytix, cambridge, MA*

ThP 483   **Characterizing the folding of recombinant therapeutic proteins by H/D exchange, native mass spectrometry and ion mobility spectrometry**; Nina Khristenko[1]; Eric Largy[1]; Jérôme Haustant[2]; Frédéric Rosu[1]; Cédric Mesmin[2]; Valérie Gabelica[1]; *[1]European Institute of Chemistry and Biology, Pessac, France; [2]Merck Biodevelopment SAS, Martillac, France*

PROTEOMICS: CLINICAL APPLICATIONS II
ThP 484-500

ThP 484   **Development of a Multivariate Model to Assess the Progression of ALS using a Peptide Signature**; Allyson L. Mellinger[1]; Emily H. Griffith[2]; Michael S. Bereman[1, 3]; *[1]Department of Chemistry, North Carolina State University, Raleigh, North Carolina; [2]Department of Statistics, North Carolina State University, Raleigh, North Carolina; [3]Department of Biological Sciences, North Carolina State University, Raleigh, North Carolina*

ThP 485   **Quantitative Proteomics Profiling of Formalin-Fixed Paraffin-Embedded (FFPE) Human Colon Pinch Biopsy for Translational Research**; Chenqi Hu[1]; Liang Jin[1]; John Maull[1]; Stephanie Gaudette[1]; Annette Schwartz Sterman[1]; Yu Tian[1]; *[1]AbbVie, Worcester, MA*

ThP 486   **Proteomics Characterization of brain extracellular vesicles in the progression of Alzheimer´s Disease**; Xavier Gallart-Palau[1, 2]; Elisabet Vilella[3]; Aida Serra[1]; *[1]+PecProteomics, IMDEA Food Research Institute,, Madrid, Spain; [2]IISPV, Hospital Universitari Institut Pere Mata, Reus, Spain; [3]IISPV, Hospital Universitari Institut Pere Mata, CIBERSAM, Reus, Spain*

ThP 487   **High Throughput Protein Quantification for Clinical Research with a New NanoLC System Coupled to a Triple Quadrupole Mass Spectrometer**; Linfeng Wu[1]; Nicolai Bache[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Evosep Biosystems, Odense, Denmark*

ThP 488   **High-content and high-throughput proteomic screening for personalized medicine using CESI-MS**; Farzin Gharahdaghi[1]; Andrea D. Matlock D. Matlock[2]; Vineet Vaibhav[2]; Simion Kreimer[2]; Jennifer Van Eyk[2]; Hans Dewald[1]; Jose-Luis Gallegos-Perez[1]; *[1]Sciex, Framingham, MA; [2]Cedars-Sinai Medical Center, Los Angeles, CA*

ThP 489   **Methionine Oxidation for Improved Multiple Reaction Monitoring (MRM) of the monoclonal antibody Bevacizumab**; Vanessa Pinatto Gaspar[1, 2]; Sahar Ibrahim[1, 2]; Vincent R. Richard[1]; Constance A. Sobsey[1, 2]; René Zahedi[1]; Christoph H. Borchers[1, 2, 3]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [2]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [3]Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

ThP 490   **Quantitative proteomics analysis of distant metastatic breast cancer using formalin-fixed paraffin-embedded (FFPE) tissues**; Dongyoon Shin[1]; Joonho Park[2]; Dohyun Han[3]; Jihye Moon[4]; Hansuk Ryu[4]; Youngsoo Kim[1]; *[1]Department of Biomedical Sciences, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea; [2]Department of Biomedical Engineering, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea; [3]Biomedical Research Institute, Seoul National University Hospital, 101 Daehak-ro Chongno-ku, South Korea; [4]Department of Pathology, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea*

ThP 491   **Development of Multiple Reaction Monitoring (MRM) Methods for Therapeutic Drug Monitoring of Monoclonal Antibodies**; Vanessa Pinatto Gaspar[1, 2]; Sahar Ibrahim[1, 2]; Constance A. Sobsey[1, 2]; Vincent R. Richard[1]; Shaun Eintracht[3]; René Zahedi[1]; Christoph H. Borchers[1, 2, 4]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [2]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [3]Department of Diagnostic Medicine, Jewish General Hospital, Montreal, Canada, Montreal, QC; [4]Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia*

ThP 492   **Proteomic analysis of low abundance IgA1-immune complexes in the serum of IgA Nephropathy patients**; Mary A. Bunten[1]; Amanda Proper[1]; Audra A. Hargett[1]; Stacy Hall[1]; Bruce A. Julian[1]; Jan Novak[1]; Matthew B. Renfrow[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

ThP 493   **Characterization of single-shot plasma proteomics performance using the PASEF method and systematic investigation into the quantitative proteome depth**; Stephanie Kaspar-Schoenefeld[1]; Thomas Kosinski[1]; Romano Hebeler[1]; Verena Tellstroem[1]; Markus Lubeck[1]; Henning Meyer[1]; Peter Brechlin[1]; Kristina Marx[1]; Pierre-Olivier Schmit[2]; Scarlet Koch[1]; Matt Willetts[3]; Dirk Wunderlich[1]; Nagarjuna Nagaraj[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonique S.A., Wissembourg, France; [3]Bruker Scientific LLC, Billerica, MA*

ThP 494   **Deep Serum Proteomics – Impact on sample processing and library approaches on the quantifiable proteome**; Raphael Heilig[1]; Georgina Berridge[1]; Philip Charles[1]; Roman Fischer[1]; *[1]University of Oxford, UK, Oxford, United Kingdom*

ThP 495   **Exploring in depth brain proteome of Alzheimer's disease (AD) with MALDI Imaging Mass Spectrometry in combination with shotgun proteomics**; Yumiko Toyama[1]; Hongsun Park[2]; Ryo Kajita[3]; Nobuto Kakuda[1]; Tomohiro Miyasaka[1]; Takashi Nirasawa[3]; Shigeo Murayama[4]; Nobuyuki Nukina[2]; Yasuo Ihara[2]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyotanabe, Japan; [2]Graduate School of Brain Science, Doshisha University, Kyotanabe, Japan; [3]Bruker Japan K.K., Yokohama, Japan; [4]The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Japan*

ThP 496   **Multiple Reaction Monitoring based targeted proteomics to screen protein biomarkers in Brain tumors**; Saicharan Ghantasala[1]; Nikita Gahoi[1]; Shuvolina Mukherjee[1]; Sanjeeva Srivastava[1]; *[1]IIT Bombay, Mumbai, India*

ThP 497   **A high-throughput platform for proteome and phospho-proteome profiling of matching tumor and adjacent normal tissue samples from thousands of patients**; Jakob Vowinckel[1]; Karel Novy[1]; Thomas Corwin[2]; Tobias Treiber[1]; Vito Dozio[1]; Roland Bruderer[1]; Lukas Reiter[1]; Eike-Christin Von Leitner[2]; Oliver Rinner[1]; Claudia Escher[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Indivumed GmbH, Hamburg, Germany*

ThP 498   **Characterization of a SP3 Method for Streamlined Urine Proteomics**; Pamela S. Cantrell[1]; Xuemei Zeng[1]; Matthew V. Fagerburg[2]; Yang Liu[1]; Nathan A. Yates[1, 2]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

ThP 499   **Molecular dissection of renal amyloidosis with MALDI - Imaging Mass Spectrometry and shotgun proteomics on paraffin embedded biopsy tissue section**; Yume Mukasa[1]; Jean-paul Duong van Huyen[2]; Marion Rabant[2]; Ryo Kajita[3]; Takashi Nirasawa[3]; Yumiko Toyama[1]; Megumi Terada[1]; Patrick Bruneval[4]; Hatsue Ishibashi-Ueda[5]; Hironobu Naiki[6]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyotanabe, Japan; [2]Necker-Enfants malads Hospital, Paris, France; [3]Bruker Japan K.K., Yokohama, Japan; [4]Georges-Pombidou European Hospital, Anatomy-Pathology, Paris, France; [5]National Cerebral and Cardiovascular Center, Suita, Japan; [6]Department of Molecular Pathology, Faculty of Medical Sciences, University of Fukui, Fukui, Japan*

ThP 500   **Affordable automated proteomics and multiomics sample preparation**; Richard Lam[1]; John Wilson[2]; John Laycock[1]; *[1]Tecan SP, Inc., Baldwin Park, California; [2]ProtiFi, LLC, Farmingdale, New York*

PROTEOMICS: QUANTITATIVE III
ThP 501-519

ThP 501   **Multi-omic characterisation reveals proteome specific trans effects in autosomal chromosomes correlating with erosion of X chromosome inactivation**; Alejandro J Brenes[1]; Harunori Yoshikawa[1]; Dalila Bensaddek[2]; Bogdan Mirauta[3]; Daniel Seaton[3]; Hao Jiang[1]; Jens L Hukelmann[4]; Angus I Lamond[1]; *[1]University of Dundee, Dundee, United Kingdom; [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia; [3]European Bioinformatics Institute, Cambridge, United Kingdom; [4]Immatics, Tuebingen, Germany*

ThP 502   **Quantitative, deep proteomics of precision therapeutics in breast cancer**; Michael J Emanuele[1]; Laura E Herring[1]; Natalie K Barker[1]; Xianxi Wang[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 503   **Comprehensive identification of HSP70/HSC70 Chaperone Clients in Human Cells**; Seung Woo Ryu[1, 2]; Rose Stewart[1, 2]; Chase Pectol[3]; Nicolette Ender[1, 2]; Oshadi Wimalarathne[1, 2]; Ji-Hoon Lee[1, 2]; Carlos P. Zanini[4]; Antony Harvey[5]; Jon Huibregtse[1]; Peter Mueller[4]; Tanya T. Paull[1, 2]; *[1]The Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX; [2]The Howard Hughes Medical Institute, The University of Texas at Austin, Austin, TX; [3]The Department of Chemistry, Texas A&M University, College Station, TX; [4]Department of Statistics & Data Sciences, University of Texas at Austin, Austin, TX; [5]Thermo Fisher Scientific, Austin, TX*

ThP 504   **Protein Profiling Confirms Inhibition of Protein Synthesis/Translation Initiation during Exposure to Sorafenib, an Inducer of Ferroptotic Cancer Cell Death**; Emily G. Werth[1, 2]; Presha Rajbhandari[1]; Prashant Kaushik[1]; Brent R. Stockwell[1]; Lewis M. Brown[1]; *[1]Columbia University, New York, NY; [2]Present address: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

ThP 505   **Label-free Quantitative Serum Proteomics Reveals Mechanistic Insights into Susceptibility to Infection after Thermal Injury**; Abby Chiang[1]; Ajitha Thanabalasuriar[2]; Margarita Camara[2]; Ashley Keller[2]; Raghothama Chaerkady[1]; Chelsea Boo[1]; Antonio Digiandomenico[2]; Sonja Hess[1]; *[1]R&D, AstraZeneca, Gaithersburg, MD; [2]BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD*

ThP 506   **Space Travel, Radiation and Human Health: Proteins Secreted by Vasculature under Low Dose Galactic Cosmic Ray Simulation**; Jayanta Chakrabarty[1]; Hazeem L. Okunola[2]; Shahar Goeta[1]; Emily G. Werth[1, 3]; Lewis M. Brown[1]; Peter W. Grabham[2]; *[1]Columbia University, New York, NY; [2]Columbia University Irving Medical Center, New York, NY; [3]Present address: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

ThP 507   **Infrared Laser Ablation Sampling for Micro-volume Proteomics**; Chao Dong[1]; Luke Richardson[2]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

ThP 508   **Investigation of hypoxia and calcineurin inhibition-induced global phosphoproteome changes in human RAMOS B cells**; Shichen Shen[1]; Shannon P. Hilchey[2]; Sailee Rasam[1]; Mutka G. Palshikar[1]; Jason Emo[2]; Juilee Thakar[2]; Martin Zand[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]University of Rochester, Rochester, NY*

ThP 510   **Mouse Quantitative Proteomics Knowledgebase: assays and protein abundance reference ranges in 20 tissues and 3 mouse strains using MRM**; Yassene Mohammed[1, 2]; Pallab Bhowmick[1]; Sarah A. Michaud[1]; Helena Pětrošová[1]; David R Goodlett[3, 4]; Christoph H. Borchers[1, 5, 6, 7]; *[1]University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC; [2]Leiden University Medical Center, Leiden, Netherlands; [3]University of Maryland, Baltimore, Baltimore, MD; [4]University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [6]Proteomics Centre, Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, Quebec; [7]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, Quebec*

ThP 512 **SLIM-labeling: principles, data processing workflows and applications in quantitative proteomics**; Nicolas Senecaut[1]; Gelio Alves[2]; Hendrik Weisser[3]; Laurent Ligniere[1]; Samuel Terrier[1]; Lilian Yang-Crosson[1]; Pierre Poulain[1]; Gaelle Lelandais[4]; Yi-Kuo Yu[2]; Jean-Michel Camadro[1]; *[1]Institut Jacques Monod CNRS, Paris, France; [2]NIH, Bethesda, Maryland; [3]Storm Therapeutics, Cambridge, United Kingdom; [4]Institut de Biologie Integrative de la Cellule, Orsay, France*

ThP 513 **Parallel reaction monitoring is a crucial tool to show a shift in myosin heavy chain isoforms in hypertrophic cardiomyopathy patients**; Cinzia Magagnotti[1]; Maria Lombardi[2]; Chiara Foglieni[1]; Annapaola Andolfo[1]; Paolo G. Camici[1, 3]; *[1]OSR, Milan, Italy; [2]OSR, Milan, Italy; [3]Vita-Salute University, Milano, Italy*

ThP 514 **Impaired Degradation Dynamics of the SNARE complex in the APP KI Mouse Model for Alzheimer's Disease**; Nalini R Rao[1]; Timothy Hark[1]; Jeffrey Savas[1]; *[1]Northwestern University, Chicago, IL*

ThP 515 **TWEAK/Fn14 Signaling Induces Synaptic Phosphoprotein Changes in Mouse Brain**; Rong-Fang Gu[1]; David Nagy[1]; Benbo Gao[1]; Christopher Hinckley[1]; Linda Burkly[1]; Ru Wei[1]; *[1]Biogen, Cambridge, MA*

ThP 516 **Comparison of MS2 and Real-Time Search MS3 Analyses for Lung Proteomes of Hydrogen Sulfide Treated Swine**; Qin Fu[1]; Zhen Liu[2]; Ruchika Bhawal[1]; Elizabeth Anderson[1]; Robert Sherwood[1]; Xiangfang Tang[2]; Hongfu Zhang[2]; Sheng Zhang[1]; *[1]Cornell University, Ithaca, NY; [2]Chinese Academy of Agricultural Sciences, Beijing, China*

ThP 517 **Proteomic analysis of C. elegans to decipher specific activation mechanisms associate with the pharmacological activation of vanilloid receptors**; Jennifer Ben Salem[1]; Bruno Nkambeu[1]; Dina N Arvanitis[2]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC; [2]Université de Toulouse, Toulouse, France*

ThP 518 **Development of non-human dynamic range standard for proteomic quantification applications**; Judy Boland[1]; Amber Henry[1]; Pegah Jalili[1]; Kevin Ray[1]; Jeffrey Turner[1]; *[1]MilliporeSigma, St. Louis, MO*

ThP 519 **Novel Regulators in TNF-α Mediated Insulin Resistance Elucidated by Quantitative Proteomic Analysis**; Rodrigo Mohallem[1]; Uma K Aryal[1]; *[1]Purdue University, West Lafayette, IN*

PROTEOMICS: TISSUE
ThP 520-543

ThP 520 **Investigation of Induction of Xenobiotic Metabolising Enzymes in a 3D Skin Model by using Proteomics and western blotting techniques**; Hatem Ali H Sallem[1]; Catherine Duckett[2]; Vikki A Carolan[3]; Tanya Klymenko[3]; Malcolm R Clench[4]; *[1]Sheffield Hallam University, SHEFFIELD, United Kingdom; [2]Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom; [3]Sheffield Hallam University, SHEFFIELD, United Kingdom; [4]Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom*

ThP 521 **Proteome responses to intermittent fasting across multiple adipose tissue depots**; Dylan J Harney[1]; Michelle Cielesh[1]; Kieren Young[1]; Mark Larance[1]; *[1]University of Sydney, Camperdown, Australia*

ThP 522 **Protein changes across lactation in the milk of a lowland gorilla and a Bornean orangutan**; Timothy Cleland[1]; Michael L Power[2]; *[1]Smithsonian Museum Conservation Institute, Suitland, MD; [2]Smithsonian Conservation Biology Institute, Washington, DC*

ThP 523 **Development of a reliable protein marker panel for evaluation of intracellular contamination in interstitial fluid extraction using high-resolution LC-MS**; Min Ma[1, 2]; Shichen Shen[1, 3]; Shihan Huo[1]; Ming Zhang[1, 3]; Yang Qu[3]; Xiaoyu Zhu[1]; Chao Xue[1]; Anthony Vu[1]; Xinxin Yang[1]; Shuo Qian[1, 2]; Qingqing Shen[1]; Jun Qu[1, 3]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Institute, Buffalo, NY; [3]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

ThP 524 **Deep-ultraviolet Laser Ablation Sampling for Localized Proteomic Analysis of Tissue**; B. Chisom Egbejiogu[1]; Remilekun O. Lawal[1]; Luke Richardson[2]; Fabrizio Donnarumma[1]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

ThP 526 **Proteomics analysis of Neural Crest cells in a developing Xenopus embryo**; Leena Pade[1]; Jaeho Yoon[2]; Dr. Ira Daar[2]; Dr. Peter Nemes[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; [2]Cancer & Developmental Biology Laboratory, National Cancer Institute, NIH, Frederick, MD*

ThP 527 **Spatially-resolved, 3D-printed Micro-sampling Coupled to Sensitive Nano-LC-MS to accurately image the protein distributions in tissues**; Ming Zhang[1]; Min Ma[1]; Shihan Huo[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

ThP 528 **in depth Proteomics of Hair Follicles of whiskers from W mutant mice clarifies KIT restriction on hematopoiesis and melanogenesis**; Mayuka Kosugi[1]; Kazuo Kinoshita[2]; Takashi Nirasawa[3]; Ryo Kajita[3]; Nobuto Kakuda[4]; Masaya Ikegawa[4]; *[1]Doshisha University, Kyotanabe City, Kyoto, Japan; [2]Shiga Medical Center Research Institute, Moriyama, Japan; [3]Bruker Japan K.K., Yokohama, Japan; [4]Doshisha University, Kyotanabe, Japan*

ThP 529 **Streamlined sample processing coupled to PASEF strategy for in-depth proteome quantification**; Fabian Hosp[1]; Katrin Hartinger[1]; Sebastian Johansson[1]; Nils A. Kulak[1]; Sophia Doll[2]; Lisa Schweizer[3]; Matthias Mann[3]; Nagarjuna Nagaraj[4]; *[1]PreOmics GmbH, München, Germany; [2]OmicEra Diagnostics GmbH, Planegg/Martinsried, Germany; [3]Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; [4]Bruker Daltonic GmbH, Bremen, Germany*

ThP 530   **High throughput, spatially-resolved proteomic analysis of a human brain tumour**; Simon Davis[1]; Connor Scott[2]; Benedikt Kessler[1]; Olaf Ansorge[2]; Roman Fischer[1]; [1]*Target Discovery Institute, University of Oxford, Oxford, United Kingdom;* [2]*Nuffield Department of Clinical Neurosciences, Oxford University, Oxford, United Kingdom*

ThP 531   **PROTEIN NETWORKS AND ASSOCIATED BIOLOGICAL PROCESSES IMPACTED IN THE GLAUCOMATOUS RETINA AND OPTIC NERVE OF ESTROGEN-DEPRIVED RATS**; Khadiza Zaman[1]; Vien Nguyen[1]; Katalin Prokai-Tatrai[1]; Laszlo Prokai[1]; [1]*University of North Texas Health Science Center, Fort Worth, TX*

ThP 532   **Supervised and Unsupervised Approaches for Multivariate Proteomic Classification and Characterization of Spatially Targeted Tissue Substructures**; Kavya Sharman[1, 2]; Nathan Heath Patterson[1, 3]; Danielle B Gutierrez[1, 3]; Elizabeth K Neumann[1, 3]; Emma R Guiberson[1, 4]; Andy Weiss[5]; William J. Perry[1, 4]; Daniel J Ryan[1, 4]; Raf Van de Plas[6]; Eric P Skaar[5]; Richard M Caprioli[1, 3, 4, 7, 8]; Jeffrey M Spraggins[1, 3, 4]; [1]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205;* [2]*Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [5]*Department of Pathology Microbiology and Immunology, Vanderbilt University, Nashville, TN;* [6]*Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands;* [7]*Department of Medicine, Vanderbilt University, Nashville, TN;* [8]*Department of Pharmacology, Vanderbilt University, Nashville, TN*

ThP 533   **Cardiac sensory afferents differentially modulate susceptibility to depression and anxiety in a mouse model of chronic heart failure**; Jennifer Ben Salem[1, 2]; Marc Kermorgant[2]; Jason Iacovoni[2]; Lionel Dahan[2]; Denis Calise[2]; Anne Pavy La-Troan[2]; Francis Beaudry[1]; Dina N Arvanitis[2]; [1]*Universite de Montreal, St-Hyacinthe, QC;* [2]*Université de Toulouse, Toulouse, France*

ThP 535   **An Optimized Sample Preparation Method of Formalin-Fixed Paraffin-Embedded Tissues for Mass Spec Applications**; Kara Zehr[1]; Bhavin Patel[2]; Amarjeet Flora[2]; Jensen Penny[2]; Sergei Snovida[2]; Ryan Bomgarden[3]; [1]*University of Illinois at Urbana-Champaign, Urbana, IL;* [2]*Thermo Fisher Scientific, Rockford, IL;* [3]*ThermoFisher Scientific, Rockford, IL*

ThP 536   **Mitochondrial ATP synthase subunit c biogenesis revealed by quantitative MS interactomics**; Marek Vrbacky[1]; Aleksandra Markovic[1]; Josef Houstek[1]; Tomas Mracek[1]; [1]*Institute of Physiology, Czech Academy of Sciences, Prague, Czech Republic*

ThP 537   **Accurate Identification and Quantification of Hydroxyproline Modified Peptides in the Extracellular Matrix of Tissues**; Brian L Frey[1]; Zach Rolfs[1]; Michael R Shortreed[1]; Yoshitaka Kawai[2]; Lei Lu[1]; Nathan V Welham[2]; Lloyd M Smith[1]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Surgery, University of Wisconsin-Madison, Madison, WI*

ThP 538   **Proteogenomics identifies novel biological effects of schizophrenia risk loci**; Matthew L Macdonald[1]; Lora Mcclain[1]; Lambertus Klei[1]; Megan Garver[1]; David Lewis[1]; Robert Sweet[1]; Nathan Yates[1]; Bernie Devlin[1]; [1]*University of Pittsburgh, Pittsburgh, PA*

ThP 539   **Method for comprehensive proteomic analysis of FFPE tissues for potential clinical utilization**; Amanda Lorentzian[1]; Enes Ergin[2]; Jonathan Bush[2]; Chinten James Lim[2, 3]; Gregor S.D Reid[2, 3]; Christopher A Maxwell[3, 4]; Philipp Lange[2, 3, 4]; [1]*Department of Cell and Developmental Biology, University of British Columbia, vancouver, British Columbia;* [2]*Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, British Columbia;* [3]*Department of Pediatrics, University of British Columbia, Vancouver, British Columbia;* [4]*Michael Cuccione Childhood Cancer Research Program, BC Children's Hospital, Vancouver, British Columbia*

ThP 540   **Quantification of Over 10,000 Proteins from 79 Mouse Tissue Types in Four Age Groups using PulseDIA Uncovers Critical Ageing Pathways**; Tian Lu[1]; Liujia Qian[1]; Wei Liu[1]; Qiushi Zhang[1]; Weigang Ge[1]; Yi Zhu[1]; Tiannan Guo[1]; [1]*Westlake University, Hangzhou, China*

ThP 541   **First Draft of the In Vivo Beta Cell Proteome by Cell Type Specific Proximity Biotinylation in BirA* Mice**; Shiva Ahmadi[1]; Elham Pourbarkhordariesfandabadi[1]; Kenichi Kimura[2]; Angela Egert[3]; Martin Breitbach[2]; Caroline Geissen[2]; Michael Hesse[2]; Robert Hardt[1]; Hubert Schorle[3]; Bernd K Fleischmann[2]; Volkmar Gieselmann[1]; Dominic Winter[1]; [1]*Institute for Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany;* [2]*Institute for Physiology 1, University of Bonn, Bonn, Germany;* [3]*Institute for Developmental Pathology, University of Bonn, Bonn, Germany*

ThP 542   **In-depth proteome profiling of breast cancer formalin-fixed paraffin-embedded tissue for early distant metastasis**; Hyeyoon Kim[1, 2]; Hophil Min[3]; Hansuk Ryu[1, 4]; Dohyun Han[2, 4]; [1]*Department of Pathology, Seoul National University College of Medicine, Seoul, South Korea;* [2]*Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea;* [3]*Doping Control Center, Korea Institute of Science and Technology (KIST), Seoul, South Korea;* [4]*Seoul National University Hospital, Seoul, South Korea*

ThP 543   **Comprehensive characterization of the phosphoproteome of gastric cancer from endoscopic biopsy specimens**; Jun Adachi[1]; Yuichi Abe[1]; Hidekazu Hirano[2]; Hirokazu Shoji[2]; Asa Tada[1]; Junko Isoyama[1]; Akemi Kakudo[1]; Daigo Gunji[1, 3]; Kazufumi Honda[4]; Narikazu Boku[2]; Tomonaga Takeshi[1]; [1]*National Institutes of*

*Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; [2]National Cancer Center Hospital, Tokyo, Japan;
[3]Kyoto University, Kyoto, Japan; [4]National Cancer Center Research Institute, Tokyo, Japan*

PROTEOMICS: TOP DOWN ANALYSIS II
ThP 544-561

ThP 544   **Improving CZE-MS/MS for both denaturing and native top-down proteomics**; Xiaojing Shen[1]; Tian Xu[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

ThP 545   **Large-scale top-down proteomics of human colorectal cancer cell lines using multidimensional separation coupled to capillary zone electrophoresis-tandem mass spectrometry**; Eli Mccool[1]; Liangliang Sun[2]; Amanda Hummon[3]; Nicole Beller[3]; [1]*Michigan State University, East Lansing; [2]Michigan State University, East Lansing, MI; [3]The Ohio State University, Columbus, OH*

ThP 546   **Assessing Regional Heterogeneity of Sarcomeric Proteoforms in Human Hearts by Top-Down Proteomics**; Elizabeth F Bayne[1]; Stanford Mitchell[1]; Trisha Tucholski[2]; Hannah Karp[1]; Max Wrobbel[1]; Yang Hu[1]; Sean Mcilwain[1]; Kosake Ujihira[1]; Joshua Hermsen[1]; Ying Ge[1]; [1]*University of Wisconsin - Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

ThP 547   **Capillary isoelectric focusing-tandem mass spectrometry for large-scale qualitative and quantitative top-down proteomics**; Tian Xu[1]; Xiaojing Shen[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

ThP 548   **Top-down analysis of intact antibodies under denatured and native conditions on the omnitrap platform coupled to an Orbitrap Mass Spectrometer**; Mariangela Kosmopoulou[1]; Athanasios Smyrnakis[1, 2]; Dimitris Papanastasiou[1]; Kyle L. Fort[3]; Alexander A. Makarov[3]; Roman Zubarev[4]; [1]*Fasmatech, Athens, Greece; [2]Institute of Nanoscience and Nanotechology, NCSR, Demokritos, Athens, Greece; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Karolinska Institute, Solna, Sweden*

ThP 549   **Real-time Instrument Control Improves Precursor Selection and Increases Proteoform Identifications in Top-down Mass Spectrometry**; Lei Lu[1]; Michael R. Shortreed[1]; Mark Scalf[1]; Lloyd M Smith[1]; [1]*University of Wisconsin-Madison, Madison, WI*

ThP 550   **A Novel Top-Down Proteomics Method Empowered by Photocleavable Surfactant and Hydrophilic Interaction Chromatography for Comprehensive Analysis of Phospholamban Proteoforms**; Austin Carr[1]; Kyle Brown[1]; Andrew Alpert[2]; Song Jin[1]; Ying Ge[1, 3, 4]; [1]*Chemistry Department University of Wisconsin-Madison, Madison, WI 53705; [2]PolyLC Inc., Columbia, MD; [3]Human Proteomics Program, School of Medicine and Public Health, Madison, WI; [4]Department of Cellular and Regenerative Biology-University of Wisconsin-Madison, Madison, WI*

ThP 551   **Efficient phosphoprotein enrichment using novel Ti-IMAC magnetic microspheres for top-down proteomics**; Qianyi Wang[1]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI*

ThP 552   **Optimized RAS top-down proteomic assay reveals expanded proteoform landscape in malignant cells**; Kanika Sharma[1]; Dominic Esposito[1]; Anna Maciag[1]; Dwight Nissley[1]; Frank Mccormick[1, 2]; Caroline Dehart[1]; [1]*NCI RAS Initiative, Cancer Research Technology Program, Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Cancer Center, UCSF, San Francisco, CA*

ThP 553   **Protein-grade FTMS Isotopic Simulator to guide the experiment design and data analysis in top-down proteomics**; Yury O. Tsybin[1]; Anton N. Kozhinov[1]; Natalia Gasilova[2]; Laure Menin[2]; Konstantin O. Nagornov[1]; [1]*Spectroswiss, Lausanne, Switzerland; [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

ThP 554   **Proteoform profile of human protamines associated with fertility: a top-down approach**; Marina Gay[1]; Judit Castillo[2]; Mar Vilanova[1]; Ada Soler-Ventura[2]; Gianluca Arauz-Garofalo[1]; Laura Villarreal[1]; Ester Sánchez-Jiménez[1]; Meritxell Jodar[2]; Rafael Oliva[2]; Marta Vilaseca[1]; [1]*Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain; [2]Institut d'Investigacions Biomèdiques August Pi i Sunyer (IDIBAPS), Faculty of Medicine, University of Barcelona, and Biochemistry and Molecular Genetics Service, Hospital Clinic, Barcelona, Spain*

ThP 555   **Passive Elution of Proteins from Polyacrylamide Gels as Intact Species for Top-Down Proteomics**; David S. Butcher[1]; Ayako Takemori[2]; Nobuaki Takemori[2]; Lissa C. Anderson[1]; [1]*National High Magnetic Field Laboratory, Tallahassee, FL; [2]Proteo-Science Center, Ehime University, Matsuyama, Japan*

ThP 556   **Informatic Solution for the FAIR Storage of Experimentally Verified Proteoforms**; Ryan T Fellers[1]; Bryan P Early[1]; Joe B Greer[1]; Richard D Leduc[1]; Neil L Kelleher[1]; Paul M Thomas[1]; [1]*Northwestern University, Evanston, IL*

ThP 557   **Optimization of Quantitative Top-Down Proteomics in Complex Samples using Protein-Level Tandem Mass Tag (TMT) Labeling**; Dahang Yu[1]; Yanting Guo[1]; Kellye A Cupp-Sutton[1]; Zhe Wang[1]; Mulin Fang[1]; Xiaowen Liu[2]; Si Wu[1]; [1]*University of Oklahoma, Dept. of Chem & Biochem, Norman, OK; [2]Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN*

ThP 558　**213 nm Ultraviolet Photodissociation for the Characterization of Diselenide Bridges in Designer Selenocysteine Proteins**; Ellie C Watts[1]; Ross Thyer[1]; Andrew Ellington[1]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

ThP 559　**Top-Down Nanoproteomics Enables Comprehensive Analysis of Low-Abundance Cardiac Troponin I Proteoforms from Human Serum**; David S Roberts[1]; Timothy N Tiambeng[1]; Kyle A Brown[1]; Yanlong Zhu[2, 3]; Bifan Chen[1, 4]; Zhijie Wu[1]; Stanford Mitchell[3, 5]; Tania M Guardado-Alvarez[1]; Song Jin[1]; Ying Ge[1, 2, 3]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*Human Proteomics Program, School of Medicine and Public Health, Madison, WI;* [3]*Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI;* [4]*Genentech Inc., South San Francisco, CA;* [5]*Molecular and Cellular Pharmacology Training Program, Madison, WI*

ThP 560　**Quantitative top-down proteomics identifies novel histone H2A-variant specific C-terminal proteolysis events**; Matthew Holt[1]; Tao Wang[2]; Nicolas L. Young[2]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Baylor College of Medicine, Houston*

ThP 561　**Selective N-terminal mass defect labelling of proteins for improved de novo top-down sequencing**; Lavrentis DIMITRIOS Galanopoulos[1]; Sam Hughes[1]; Faye Cruickshank[1]; Colin Logan Mackay[1]; David Clarke[1]; [1]*University of Edinburgh, Edinburgh, United Kingdom*

SMALL MOLECULES: QUANTITATIVE ANALYSIS III
ThP 562-587

ThP 562　**A Simple and Sensitive LC-MS/MS Method for the Quantitation of Amlodipine in Human Plasma**; Junyi Yang[1]; Xianmiao Zhang[1]; Cuihan Ren[1]; Xiaonan Tang[1]; John (zhongping) Lin[1]; Luca C Matassa[1]; Mike (qingtao) Huang[2]; Sudhakar Pai[2]; [1]*Frontage Laboratories, Inc, Exton, PA;* [2]*Akros Pharma Inc., Princeton, NJ*

ThP 563　**A Novel Liposome Freeze/Thaw Stabilize Reagent and Its Application in theQuantitation of Free and Liposomal Doxorubicin in Rat Plasma**; Guoliang Zhang[1]; Sheng Wang[1]; Jing Huang[1]; Xiaoying Jin[1]; Dawei Zhou[2]; [1]*Lab Testing Division of WuXi AppTec, Inc., Suzhou Site, Suzhou, China;* [2]*WuXi AppTec, Cranbury, NJ*

ThP 564　**Extractables Detection in Rubber Plug Products**; Chang Jiang; *Agilent, Chengdu, China*

ThP 565　**Quadrupole-Linear Ion Trap (Q-LIT) Tandem Mass Spectrometry forQuantification of 25-Hydroxyvitamin D2 in Human Serum**; Jie Xie[1]; Wei Zeng[1, 2]; You Jiang[1]; Shiying Chu[1]; Guoqing Shi[2]; Xinhua Dai*[1]; Xiang Fang*[1]; [1]*Mass Spectrometry Engineering Technology Research Center, Center for Advanced Measurement Science, National Institute of Metrology, Beijing, People's Republic of China, Beijing, China;* [2]*School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing, People's Republic of China, Beijing, China*

ThP 566　**High Sensitivity Analysis of Estrogens in Human Serum, Human Urine and Environmental Water Samples without Derivatization by Direct Injection LC-MS/MS**; Jingcun Wu[1]; Saba Hariri[1]; Tyrally Ordinario[1]; Feng Qin[1]; Cheng-Yuan Cai[2]; [1]*PerkinElmer Inc., Woodbridge, ON;* [2]*PerkinElmer Management Co.,, Shanghai, China*

ThP 567　**Development of a Rapid and Simple LC-MS/MS Method for the Simultaneous Determination of Olsalazine and Mesalazine in Rat Plasma**; Mingming Wang[1]; Deping Cheng[1]; [1]*Alliance Pharma Inc, Malvern, PA*

ThP 568　**LC-MRM-MS Method for the Detection and Quantification of Six Nitrosamine Impurities in Sartan (ARBs) Drugs**; Roxana Eggleston-Rangel[1]; Phil Koerner[1]; J Preston[1]; Laura Snow[1]; [1]*Phenomenex, Torrance, CA*

ThP 569　**Determination of Pirfenidone and Metabolites in Rat Plasma by Coupling On-Line Fractionation with LC-MS/MS**; Ming-Luan Chen[1]; Jeff Plomley[1]; Milton Furtado[1]; Anahita Keyhani[1]; [1]*Altasciences, Laval , QC*

ThP 570　**Rapid, Affordable and Efficient Screening of Blood in People Exposed to Air Pollution**; Raminta Zmuidinaite[1]; Jonathan Lacey[1]; Christian Jardine[1]; Ray Iles[1]; [1]*MAP Sciences, Bedford, United Kingdom*

ThP 571　**Development and Validation a Simple and Rugged LC-MS/MS Method to Simultaneously Measure Rosuvastatin, Fexofenadine, Midazolam and Pitavastatin in Human Plasma**; Nick Peng[1]; Ardeshir Khadang[1]; [1]*Axis Clinicals, Dilworth, MN*

ThP 572　**Highly sensitive LC-MS/MS method for the determination of NDMA, NDEA, NDIPA, NMBA, NEIPA and NDBA in Metformin Drug Substance**; Shailendra anil Rane[1]; Deepti Bhandarkar[1]; Anant Lohar[1]; Bhaumik Trivedi[1]; Purushottam Sutar[1]; Ashutosh Shelar[1]; Navin Devadiga[1]; Shailesh Damale[1]; Jitendra Kelkar[1]; Ajit Datar[1]; Pratap Rasam[1]; [1]*Shimadzu Analytical (India) Pvt. Ltd, Mumbai, India*

ThP 573　**A Facile and Sensitive Method for the Quantification of Pyrrolidine in Rat Plasma Using LC-MS/MS**; Mei Sun[1]; Renmeng Liu[1]; Mingming Wang[1]; Deping Cheng[1]; [1]*Alliance Pharma, Inc., Malvern, PA*

ThP 574　**High Throughput Antiretroviral Drug Metabolite Quantitation from Small Amounts at Subtherapeutic Levels**; Farzin Gharahdaghi[1]; Craig Sykes[2]; Hans Dewald[1]; Jose-Luis Gallegos-Perez[1]; [1]*Sciex, Framingham, MA;* [2]*Division of Pharmacotherapy and Experimental Therapeutics, University of North Carolina, Chapel Hill, North Carolina*

ThP 575 **Development of a Novel Quantitative Platform for Multi-amines in Foods Using Reductive Amination Modification and Mass Spectrometry**; Shih-Shin Liang; *Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 576 **Improve sensitivity for Quantification of Antisense Oligonucleotides in Plasma Using Microflow LC-MRM Methodology**; Ji Jiang[1]; Sean Mccarthy[2]; Esme Candish[2]; Lei Xiong[1]; *[1]SCIEX, Redwood Shores, California 1201; [2]Sciex, Framingham, MA*

ThP 577 **Investigation of whole blood stability during LC-MS/MS bioanalytical method validation**; Philip S. Wong[1]; Anna Akrami; Christopher James[1]; *[1]Amgen, Thousand Oaks, CA*

ThP 578 **Development of a Data Processing Approach to Support Ultra High-Throughput MS Acquisition**; Mikael Levi[1]; Davide Vecchietti[1]; Hiroyuki Yasuda[1]; Kazuto Mannen[2]; Toru Shiohama[1]; Mitsuhiro Kanazawa[2]; Tairo Ogura[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Reifycs Inc., Tokyo, Japan*

ThP 579 **Determination of Nitrosamine impurities in Pregabalin drug substance using Triple Quadrupole Liquid Chromatography Mass Spectrometry**; Chander Mani[1]; Saikat Banerjee[2]; *[1]Agilent Technologies, Haryana, India; [2]Agilent Technologies India Pvt Ltd, Hyderabad, India*

ThP 580 **Targeted quantification of water soluble B vitamins from faba bean seeds using UPLC-SRM MS**; Jeremy DS Marshall[1]; Haixia Zhang[1]; Ambuj Jha[1]; Albert Vandenberg[1]; *[1]University of Saskatchewan, Saskatoon, SK*

ThP 581 **Quantitative LC-MS/MS Method for the Determination of Six Nitrosamines Using Isotope Labeled Standard Calibration**; Pei Wang[1]; Holly Post[1]; Thomas Leitzinger[1]; Jie Ding[1]; *[1]PPD, Inc, Middleton, WI*

ThP 582 **Overcoming data challenges in automated mass spectrometry-based screening of entire compound libraries**; Roger Ford[1]; Lope Florez[2]; Aude Tartiere[3]; Stephan Heyse[2]; *[1]Genedata, Lexington, MA; [2]Genedata AG, Basel, Switzerland; [3]Genentech Inc, South San Francisco, CA*

ThP 583 **The QTOF methodology for targeted quantitative analysis with similar sensitivity to triple quadrupole**; Bingfang Yue[1]; Loan T Nguyen[1]; Daniel M Anderson[1]; *[1]NMS Labs, Horsham, PA*

ThP 584 **Lessons Learned: Adverse Effects of In-Source Fragmentation on Quantitative Accuracy for Isomeric Mixtures in Biological Samples**; Lori L. Smith[1]; Trey A. Vinke[1]; Katherine E. Barre[1]; Kristin L. Aillon[1]; Suramya Waidyanatha[2]; Bradley J. Collins[2]; *[1]MRIGlobal, Kansas City, MO; [2]Division of National Toxicology Program, NIEHS, Research Triangle Park, NC*

ThP 585 **Quantitative analysis of N-nitrosodimethylamine in metformin tablets using liquid chromatography–high resolution mass spectrometry**; Gunwoo Kim; *Chung-ang university, Seoul, South Korea*

ThP 586 **Development of a simple, selective and sensitive bioanalytical method for the analysis of Donepezil in plasma using LC-ESI-MS/MS**; Chidella Kartheek Srinivas[1]; Prasanth Joseph[1]; Arun Kumar P[1]; Saikat Banerjee[1]; Samir Vyas[2]; *[1]Agilent Technologies, BENGALURU, India; [2]Agilent Technologies, Mumbai, India*

ThP 587 **Simultaneous Quantitation of Nicotine, Cotinine, THC and Their Glucuronide Metabolites in Human Urine by LC-MS/MS**; Moo-Young Kim[1]; Christopher Cousineau[1]; Fumin Li[1]; *[1]PPD, Middleton, WI*

WORKSHOPS

REBOOT

Live webinar workshops will be accessible to registrants of the ASMS 2020 Reboot via the mobile app and online planner. Webinars will be recorded and available on-demand to registrants. Descriptions follow this page in chronological order.

TUESDAY, JUNE 2, 10:00 - 11:30 AM

Tues-01 | **Proteoform identification and quantification using TopPIC suite**

Tues-02 | **FAIMS/DIMS/DMS Technology and its Impact on Current Day MS Analyses**

Tues-03 | **Pros and Cons of Sample Preparation in Ambient Ionization Direct Introduction Mass Spectrometry**

Tues-04 | **Tangible Tools for Expanding Diversity and Inclusion**

Tues-05 | **Bridging Native-MS in Academia and Industry: From Direct nESI Infusion to Platform Sample Introduction and Routine Project Support**

Tues-06 | **Trans-Proteomic Pipeline: Recent Advances and Future Directions**

TUESDAY, JUNE 2, 12:00 - 1:30 PM

Tues-07 | **Flavors, Fragrances and Contaminants: Getting Informatics Approaches to Work for You**

Tues-08 | **HDX, Covalent Labeling & Cross-Linking: New developments and applications**

Tues-09 | **Ion Trap Mass Spectrometry : Latest Trends in Ion Traps For Exploring Space, Other Planets, and Earth**

Tues-10 | **MS Career Options: How to Kick Start Your Career**

Tues-11 | **Metabolomics: Balancing New Research Developments and Service Core Deliverables**

WEDNESDAY, JUNE 3, 10:00 - 11:30 AM

Wed-01 | **Compound Identification by Mass Spectral Library Searching**

Wed-02 | **Multi-omics Research using Mass Spectrometry**

Wed-03 | **Networking for Scientists: Celebrating Women Mass Spectrometrists Year 3**

Wed-04 | **Machine Learning: How is it enhancing Mass Spectrometry?**

Wed-05 | **Art, Archaeology, and Paleontology**

Wed-06 | **MassIVE.quant: enabling community access to quantitative mass spectrometry data**

Wed-07 | **Extractables and Leachables Analytical Methodologies and Best Practices**

WEDNESDAY, JUNE 3, 12:00 - 1:30 PM

Wed-08 | **IM-MS technology in the industry - barriers and opportunities**

Wed-09 | **Building PUI / R1 Connections: A Win-Win for Both**

Wed-10 | **Data Independent Acquisition: Quo vadis?**

Wed-11 | **New aspects in the development of Multi-Attribute Method (MAM)**

Wed-12 | **Photoionization - Between Vacuum and Atmospheric Pressure**

Wed-13 | **The Role of the International Lipidomics Society**

Wed-14 | **Top Down Proteomics and Top Down Mass Spectrometry: Adoption and Expanding Applications**

THURSDAY, JUNE 4, 10:00 - 11:30 AM

Thurs-01 | **The NIH and NSF Review and Funding Process**

Thurs-02 | **Advances in Automation for Proteomics Sample Preparation**

Thurs-03 | **Cannabis & Hemp Mass Spec Workshop: A Closer Look at the Applications of Mass Spectrometry in Cannabis quality control, compliance and research**

Thurs-04 | **Developing World: Supporting Education and Research in Mass Spectrometry**

Thurs-05 | **The Proteomics Standards Initiative and ProteomeXchange: Supporting open data practises in the proteomics field**

Thurs-06 | **MS-Based Process Analytical Technology (PAT): Monitoring Everything from Large Molecules to Cell Therapies**

Thurs-07 | **Career Opportunities for Chinese Students and Scholars**

Thurs-08 | **Polymeric Materials Interest Group - Investigating Polymer Architecture**

THURSDAY AFTERNOON, JUNE 4, 12:00 - 1:30 PM

Thurs-09 | **Ambient Ionization: How can we make it more reproducible?**

Thurs-11 | **Machine learning analysis of mass spectrometry data in the life sciences**

Thurs-12 | **Standardizing the Imaging MS Workflow: Current Progress**

Thurs-13 | **Leveraging Emotional Intelligence Strategies during the Pandemic**

Thurs-14 | **The Multidimensional Clinical Space - From Discovery to Practice in Screening and Diagnostics**

Thurs-15 | **Large-Scale Data Analysis and Management: Challenges for Analytical Laboratories**

Tues-01
Proteoform identification and quantification using TopPIC suite
Independent

Presiders: Xiaowen Liu, Liangliang Sun, Si Wu

Top down mass spectrometry (MS) has gained increasing attention in the past decade because of its capability to sequence whole proteoforms with post-translational modifications (PTMs) and other alterations. Although many computational methods have been developed for top-down MS data analysis, it is still challenging for MS labs to efficiently identify and quantify proteoforms because of the complexity of the data and methods. TopPIC suite is an open source software package that is routinely used for proteoform identification and characterization by top-down MS. In this workshop, we will present new tools in TopPIC suite for the visualization of mass spectra and proteoform identifications. In addition, we will give tutorials on a TopPIC pipeline for proteoform identification and quantification as well as applying the tools to various research problems ranging from phosphorylated proteoform identification to native proteomics. We will discuss with users and collect their feedback and suggestions for further improvement of the tools.

Tues-02
FAIMS/DIMS/DMS Technology and its Impact on Current Day MS Analyses
Independent

Presiders: Susan Abbatiello, Pierre Thibault

The goal of this workshop is to provide a forum for people interested in High-field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) and Differential Ion Mobility Spectrometry (DIMS or DMS). We will go over the basics and fundamentals of how FAIMS/DIMS/DMS works, differences in hardware, the effects of different parameters on performance, and how it is different than Drift-Tube Ion Mobility (DT-IMS). Examples of applications benefiting from FAIMS/DIMS/DMS will be discussed, and attendees are invited to bring their questions and experiences of success, uncertainty, and even bad luck, to share with the community. Discussion will be led by several subject matter experts.

Tues-03
Pros and Cons of Sample Preparation in Ambient Ionization Direct Introduction Mass Spectrometry
Independent

Presiders: Janusz Pawliszyn, Abraham Badu-Tawiah

The main objective of the workshop is to create forum to share experience about ambient ionization direct introduction Mass Spectrometry and its performance with and without sample prep build into the procedure. Many ambient ionization procedures have incorporated the separation step resulting in some discrimination and elimination of interferences, but the effectiveness of the approaches are different. Therefore some of the techniques benefits from additional clean-up step for smore complex matrix applications. Others are designed to integrate well the clean-up with the sampling/introduction process. Discussion of important fundamentals which could lead to improvement of design of the procedures to facilitate better performance will be conducted during the workshop.

Tues-04
Tangible Tools for Expanding Diversity and Inclusion
Independent

Presiders: Jessica Prenni, Scott McLuckey, Livia Eberlin

This workshop will be facilitated by the ASMS Diversity Committee and will feature Dr. Corinne Moss-Rascusin, professor of Psychology at Skidmore College. Dr. Moss-Rascusin will also be presenting a special keynote lecture on Sunday: "Is there still gender bias in academic science (and does it matter?); what the scientific studies say". This workshop will serve as a follow-up session to her keynote lecture and will enable additional opportunity for questions and discussion. In addition, Dr. Moss-Rascusin will give a short presentation on resources that her group has created for effective interventions to reduce STEM gender bias. Specifically, her group has developed and evaluated a set of tools called VIDS (Video Interventions for Diversity in STEM), interventions derived from research in communications and the psychological literature on attitude change, persuasion, and diversity intervention efficacy. These tools are available as a free resource for the scientific community.

Tues-05
Bridging Native-MS in Academia and Industry: From Direct nESI Infusion to Platform Sample Introduction and Routine Project Support
Independent

Presiders: Iain Campuzano, Michael Marty,

Since the initial experiments performed in academia demonstrating the retention of noncovalent protein-ligand and protein-protein complexes in the gas-phase over twenty-five years ago, this unique application area of MS has grown into a fully established research field with applications for project support and progression within pharma.
The protein complexes investigated by native-MS have ranged from the initial demonstrations on simple protein complexes, through complex macromolecular machines, to the present-day analysis on polydisperse nanodiscs, membrane proteins, and mega-Dalton virus capsids.
What has remained relatively constant is sample introduction with single-shot, low-volume nanoESI capillaries. However, sample introduction for native-MS is beginning to evolve rapidly using more "platform" based technologies. There are now multiple examples within pharma, where native-MS is critical for project support and progression, but still remains niche, due to lack of robust, higher throughput introduction methods.

Within this workshop, we will discuss the diversity of samples now being analyzed by native-MS in both academia and pharma; new and evolving sample introduction methods ranging from single-shot nESI, to high-throughput automated native-MS acquisitions. Our focus is to bridge new technology and applications development in both academic and pharma research environments allowing for routine project support and progression for modalities that require native-MS analytics.
Subject matter would include:
1. Sample diversity now being analysed by native-MS; academia and industry
2. Improvements in single-shot nESI sample introduction (NanoMate and submicron emitters) and perceived challenges.
3. Platforming native-MS methods (SEC-MS and CEX-MS, ceIF-MS and HT native-MS)
4. ToF, Orbitrap, and FT-ICR as native-MS instrument platforms.

Tuesday, June 2, 10:00 - 11:30 am
Tues-06
Trans-Proteomic Pipeline: Recent Advances and Future Directions
Independent

Presiders: Michael Hoopmann, David Shteynberg,

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 topic leads for discussion are: improved label-free quantitation with StPeter, export of TPP results for the mzIdentML format, techniques for creating an abundance matrix for many samples, and spectrum-centric DIA analysis and quantitation with DISCO, including new ion mobility support. 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-07
Flavors, Fragrances and Contaminants: Getting Informatics Approaches to Work for You
Flavor Frangrance & Foodstuff Interest Group

Presiders: James Redwine, Travis Falconer,

Methods described as "non-targeted" have been a popular topic in the analysis of fragrances and foodstuffs over the past several years. Regardless of the type of mass analyzer used in these methods, the data is typically subjected to treatment utilizing an informatics approach, typically falling under descriptions such as "-OMIC," multivariate, or chemometric (among others). These approaches represent promising capabilities in analyzing a wide range of Analytical problems imposed by the typically complex matrices involved in analysis of food. However, the implementation of these techniques can be quite challenging due to steep learning curves associated with the mathematics and software.
The goal of this workshop is to demonstrate some successful applications of non-targeted analyses of food-related samples using a range of commonly available commercial software packages. Topics of interest include sample preparation techniques, instrument methodology, suggested configuration of data treatment and analyses, and choosing appropriate multivariate analysis methods and visualizations. Topics will be open to analysis related to desirable sensory attributes, undesirable sensory attributes, authentication, and contaminants of concern.
The format of the workshop will consist of a few brief presentations demonstrating successful utilization of the methodologies, followed by discussion moderated by the interest group co-chairs.

Tues-08
HDX, Covalent Labeling & Cross-Linking: New developments and applications
HDX Covalent Labeling & Cross Linking Interest Group

Presiders: James Bruce, Miklos Guttman,

Developments in MS instrumentation, sample preparation strategies, reagents and informatics tools have significantly advanced applications of HDX, covalent labeling and cross-linking approaches in protein structural and interaction analysis. This workshop will feature invited speakers with expertise in HDX, chemical labeling, and cross-linking methods to briefly introduce the technique and present recent methodology advances and exciting applications. The invited speakers will then form a panel for the second part of the workshop to address topics based on interest group feedback and moderated participant-submitted questions.

Tues-09
Ion Trap Mass Spectrometry : Latest Trends in Ion Traps For Exploring Space, Other Planets, and Earth
Ion Trap MS Interest Group

Presiders: Desmond Kaplan, Theresa Evans-Nguyen,

In honor of being in Houston, TX, the Ion Trap Interest Group Meeting will cover the latest trends in instrumentation and applications in ion trap mass spectrometry for planetary exploration both on our own planet Earth and on other planets. Instrumentation topics will cover some of the most recent instrumentation, scanning methods and applications for ion trap mass spectrometry in space flight missions. Earth instrumentation Applications will cover some of the latest instrument, ion/molecule and ion/ion reaction methods that are used to study our atmosphere, ocean bodies, and air quality. The workshop will consist of lightning-fast talks to introduce the topics and extended question and answer sessions to discuss, among other details, the limitations to commercialization of new advances.

Tues-10
MS Career Options: How to Kick Start Your Career
Young Mass Spectrometrists Interest Group

Presiders: Sharon Pitteri, Christopher Rose,

This workshop features a panel discussion on professional development in the area of mass spectrometry. Topics will be focused on career planning and management, training, internships, job search tools, and interview strategies. The panel, consisting of representatives from industrial and academic organizations, will share their experiences and knowledge and practices on career prospects.

Tues-11
Metabolomics: Balancing New Research Developments and Service Core Deliverables
Metabolomics Interest Group

Presiders: Timothy Garrett, Miriam Sindelar,

Two exciting trends are happening in metabolomics. First, the number of core facilities that offer metabolomics services is increasing rapidly. Almost every major research institution around the world now has access to metabolomics, which has helped extend metabolomics to a growing number of biological applications. Second, a stream of innovative metabolomic technologies are constantly being introduced to the community. This includes not only improvements in hardware, but also advances in software and databases. The goal of this workshop is to consider the intersection of these two trends. What services should be offered by core labs? How and when should new technologies be assimilated? How should labs deal with competing solutions to the same analytical challenges? Should metabolomic researchers be using different workflows than offered by core facilities? Key to these questions is managing the expectations of the researcher, while also maximizing the potential for discovery. The NIH metabolomics common fund has played an integral role in both supporting service cores and technology developments since 2010. These NIH initiatives will be used as a general organizational framework to facilitate discussion.

Wed-01
Compound Identification by Mass Spectral Library Searching
Independent

Presiders: Xiaoyu Yang, Stephen Stein,

Mass spectral library searching is an essential tool for the reliable identification of compounds in complex mixtures. The objective of this workshop is to provide a forum for participants to learn what a mass spectral library is, what libraries are available, how to use them, how to build their own, and problems and solutions arising when searching libraries. Workshop coordinators will first briefly introduce some fundamentals about mass spectral libraries and present an overview of the development of libraries and general principles of library searching. Then, 4-5 experts from industry and academia will briefly discuss their library-based work and plans. Discussion topics will include: 1) the available libraries, including widely used GC/MS and rapidly developing LC/MS/MS, commercial and free libraries, and associated searching software; 2) library applications in metabolomics, proteomics, lipidomics, food, and environmental studies; 3) library searching issues such as comprehensiveness of libraries, causes of false-positive identification, spectral quality, and variability of library spectra across different instruments and measurement conditions; 4) challenges and strategies for identifying compounds not in the library. The audience will be encouraged to ask questions to the presenters and share their experiences of success, tips, tricks and lessons, suggestions and concerns, problems and questions about library searching. At the end of the workshop, we hope participants will learn how mass spectral library searching can aid their discovery and confirmation of compound identity.

Wed-02
Multi-omics Research using Mass Spectrometry
Independent

Presiders: Pratik Jagtap, Susan Weintraub, Timothy Griffin

Advances in mass spectrometry (MS) based methods have enabled deeper biological insights using proteomics and metabolomics approaches. This has also resulted in improvements in our ability to compare and correlate MS data with other 'omics methods such as genomics and transcriptomics - thus enabling multi-omics research.
Experts will present their work in the area of multi-omics research – focusing on challenges and opportunities to implement these methods. Talk topics will include experiences with integrating advanced mass spectrometry technology methods and meta-omics analysis for characterizing complex microbiome. Proteogenomics talk will cover integrating diverse data types and developing statistical methods to analyze large comprehensive proteogenomics datasets. Analytical methods in genomics, epigenomics, and metabolomics to characterize disease biomarkers and therapeutic targets will also be covered.
The presentations will be followed by a panel discussion that will address the challenges and opportunities in correlating MS outputs with other multi-omics methods.

Wed-03
Networking for Scientists: Celebrating Women Mass Spectrometrists Year 3
Independent

Presiders: Anumita Saha, Erin Baker, Komal Kedia

Considering the enthusiasm for networking and feedback from participants in previous years, the third year of this workshop will focus on creating more opportunity for more one-on-one interaction with panelists. This year we will start with a short panel introduction but save the majority of the workshop time for panelists and participants to break out into small groups for more one-on-one interaction. Pre-determined topics and sample questions focusing on a range of relevant topics will be provided to encourage discussion and help the introvert in you to come out and ask. Throughout the workshop, participants will be prompted to rotate to a new panelist enabling ample opportunity for networking. The panel will consist of women in various areas (e.g. industry, academia, pharmacy, etc.) and stages of their career such that both early and mid-career professionals can benefit.

Wed-04
Machine Learning: How is it enhancing Mass Spectrometry?
Independent

Presiders: Gaurav Chopra, Graham Cooks, Hilkka Kenttämaa

Recent advances in machine learning and artificial intelligence (AI) are revolutionizing the human/technology interface. Mass spectrometry (MS) is a powerful analytical tool that is extensively used for characterization of substances and mixtures across many fields, such as chemistry, biology, pharmaceuticals, petroleum, etc. Machine learning tools are emerging to support autonomous science, in which critical decision-making on experimental design is conducted by algorithms rather than by human intervention. This shift from automation to autonomation is enabled by rapid advances in data science and deep neural networks. We will discuss several questions with selected 5 minutes of overview presented by experts in the field: How machine learning/AI algorithms is enhancing MS autonomation? Does machine learning/AI enhance analysis of ion-molecule reactions, ion-ion reactions, multiple reaction monitoring, nano-DESI, proteomics, metabolomics, lipidomics, etc? How does chemical representation affect MS analysis and results? What are the current challenges in MS methods that machine learning/AI can and cannot address? Is it possible to develop an autonomous methodology that can be easily implemented into commercial mass spectrometers with only minor instrument modifications? Can we develop machine learning methods that are understandable by human chemists for decision making? Are there specific deep learning architectures that work better than others for identifying structure from spectra? Do we need MS scientists trained in data science to handle the exponential increase in data obtained using mass spectrometry? Our workshop will address revolutionary changes in data science and artificial intelligence that may result in new opportunities at the interface between data and MS based measurement science.

Wed-05
Art, Archaeology, and Paleontology
Independent

Presiders: Enrico Cappellini

Mass spectrometry allows confident identification of organic and inorganic compounds present at low abundance in complex mixtures that originate from artistic, archeological and paleontological remains.
This well-established, robust and reliable approach has already provided very innovative results in the study, diagnostics and protection of cultural heritage collections. Similarly, mass spectrometry enabled recovery of genetics information much older than previously achieved by other techniques. Accordingly this technique is becoming instrumental to address a wide range of outstanding questions pertaining to the deep-time evolutionary history of multiple animal, including human, species.
This workshop aims at sharing experience on innovative and advanced methods for sample preparation, mass spectrometry measurement and automated data analysis, focusing in particular on the challenging specificities of cultural heritage materials.

Wed-06
MassIVE.quant: enabling community access to quantitative mass spectrometry data
Independent

Presiders: Olga Vitek

MassIVE.quant is a new tool-independent repository infrastructure and data resource for community sharing of reproducible quantitative mass spectrometry-based biomedical research. MassIVE.quant supplements the raw experimental data with detailed annotations of the experimental design, analysis scripts, and results, which enable the quantitative interpretation of mass spectrometry-based experiments and the online interactive exploration of the results. Aiming to support the MS community with an open platform based on open standards for data sharing MassIVE.quant is independent of data acquisition types, and of computational tools used to complete the analyses. Short use cases will be described to exemplify the utility of storing, sharing, reanalyzing, and curating data from quantitative experiments, including proteomic datasets from benchmark controlled mixtures and biological investigations, interpreted with various data processing tools and analysis options. After briefly illustrating the goals of the MassIVE.quant platform with common use cases, the workshop will focus on the open discussion of features, data and accessibility standards that would best meet the research needs of mass spectrometry research labs attempting to share or reuse quantitative MS data in the public domain.

Wed-07
Extractables and Leachables Analytical Methodologies and Best Practices
Independent

Presiders: Kate Comstock, Gyorgy Vas,

Mass spectrometry plays an essential role in extractable and leachable (E&L) analysis. Complete E&L profiles require GC-MS, LC-MS, and ICP-MS analysis. The advancements in mass spectrometry instrumentation and new techniques provide new and much-needed tools for confident and comprehensive E&L profiling.

Currently, the increasing demands for E&L analysis are driven by growth in medical devices, single-use systems (SUS), continuous processing in bioproduction, etc. The variation in materials, applications, and interactions with contact media of these products pose new challenges for E&L analysis. Furthermore, the existing E&L regulations are lacking in clarification of acceptance for these new products.

There are many techniques and new developments for E&L analysis in terms of sample preparations, chromatographic separations, and data acquisitions by various mass spectrometry instruments. In addition, the data processing and interpretation often are rate-limiting factors, and there is an urgent need for efficient, easy-to-use data processing software, E&L database and spectral libraries, and result reports generator.

This workshop will provide a venue for E&L analysis scientists to discuss all the above issues, exchange practices, also present problems and challenges concerning mass spectrometry instrumentation, methodologies, and data processing.

Through this workshop, E&L scientists will have direct open discussion and information exchange, establish and expand networks. It will promote good science and advancement of mass spectrometer's usage in E&L analysis.

Wed-08
IM-MS technology in the industry - barriers and opportunities
Ion Mobility MS Interest Group

Presiders: Jakub Ujma, Ian Webb, Kelly Hines

IM-MS technology in the industry - barriers and opportunities
The availability of commercial instrumentation and continuous improvements in technology have led to the adoption of IM-MS in fields benefiting from complex samples and complex mixture analyses. The latter statement is particularly true for academic labs and discovery led R&D; in other words, promising proof-of-principle experiments have been demonstrated but not always followed by implementation of IM-MS as a routine technique in an industrial setting. In this year's workshop, we attempt to explore the origins of this situation. We invite colleagues from several industries to share their views on IM-MS technology in their companies. A range of IM-MS applications will be highlighted, ranging from the small molecule, -omics to polymers and structural characterization of intact proteins. Presenters will be asked to contrast IM-MS with a competing analytical technique. Following a short (5 min) presentations, the session will take the form of a panel discussion. We hope to uncover issues that currently impede wider adoption of IM-MS, such as cost, the complexity of underlying physical phenomena, instrument ease-of-use, performance as well as challenges related to available software packages and data analysis. Workshop organizers anticipate that such discussion will help to identify areas where impact can be made. Thus, the workshop will provide a forum for industrial scientists to express their valued feedback, which, in turn, will benefit the community developing the IM related technology, methods, and software.

Wed-09
Building PUI / R1 Connections: A Win-Win for Both
Undergraduate Research in MS Interest Group

Presiders: Jay Forsythe, Kate Stumpo,

This workshop will provide networking opportunities for faculty at primarily undergraduate (PUI) institutions and faculty at PhD-granting (R1) institutions. For PUI faculty, gaining low-cost (or free) access to advanced MS instrumentation can be difficult but is often necessary to maintain a successful research program. For R1 faculty, connecting with research-active PUIs is advantageous in order to recruit high-quality graduate students with MS experience and to satisfy broader impacts or educational criteria in grant proposals. The workshop will begin with a group discussion of ideas and strategies for collaboration and will then break out into unstructured time for networking.

Wed-10
Data Independent Acquisition: Quo vadis?
Data Independent Acquisition Interest Group

Presiders: Birgit Schilling, Florian Meier,

In recent years, data independent acquisition (DIA) schemes have become increasingly popular as they promise high levels of reproducibility and data completeness in large sample cohorts, suitable for systems biology and translational research.
In DIA, the mass spectrometer cycles through pre-defined precursor mass windows for fragmentation and mass analysis. Tracing of fragment ion signals results in precise quantification similar to SRM/PRM, while wide precursor mass windows ensure broad analyte coverage and enable high-throughput workflows. The latter results in highly complex fragment ion spectra, which present a formidable challenge for computational analysis. Most current workflows employ spectral libraries to extract quantitative signals from as many analytes as possible. New developments address challenges in selecting optimal transitions and increase the robustness of scoring models. While these strategies require the acquisition of a spectral library in the first place, the adaptation of deep learning may render this step superfluous by generating in silico libraries. Computational advances also make entirely library-free approaches increasingly attractive. DIA greatly benefits from technological advances in the latest generation of mass spectrometers. The implementation of ion mobility has the potential to further improve speed and sensitivity. Even though most current DIA applications focus on label-free whole proteome quantification, the analysis of post-translational modifications or small molecules has also become more popular.
In this workshop, we invite experts in the field to discuss technological and software innovations, as well as promising biological and medical applications. The open format should engage discussions about unique challenges, but also opportunities for future developments.

Wed-11
New aspects in the development of Multi-Attribute Method (MAM)
Biotherapeutics Interest Group

Presiders: Hao Zhang, Rich Rogers, Da Ren

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 and electrophoretic testing methods for monitoring both product and process quality attributes (Rogers et al., AAPS J, 2017). As we enter a new decade of technology and method development, MAM and its original initiation of MS in QC are facing many new aspects. 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/multiple enzyme digestion approaches, subunit analysis-based MAM, fully automatic sample preparation, compact MS for MAM in QC and new data acquiring approaches like PRM are presented recently. The biotherapeutic interest group workshop offers a forum for members to share and discuss those new aspects in the development of MAM.

Wed-12
Photoionization - Between Vacuum and Atmospheric Pressure
Photoionization MS Interest Group

Presiders: Matthias Lorenz, Luke Hanley, Sven EHLERT

Photoionization mass spectrometry covers a wide range of techniques and methods. The most obvious differentiation here is certainly the classification between vacuum and atmospheric pressure techniques but there are many other aspects that could be used to group the existing techniques. In this year's workshop, we want to take the time to structure the variety and discuss applications.
Two experts in the areas of vacuum and atmospheric pressure photoionization will introduce their respective work to illustrate the diversity of techniques that are combined under the topic of photoionization mass spectrometry. The short presentations are expected to initiate a lively discussion and we plan to open the floor specifically to the audience to enable further contributions. In the last years we always observed an interest of participants to get in contact and discuss with experts. Since this interaction is an essential function of the photoionization interest group, there will also be a corresponding time window for this in the workshop.

Wed-13
The Role of the International Lipidomics Society
Lipids & Lipodomics Interest Group

Presiders: Kim Ekroos, Michal Holcapek,

The field of lipidomics is rapidly evolving and offers new opportunities for studying the roles of lipids in cellular biology as well as in health and disease. This is driven by the emergence of modern mass spectrometric technologies providing extended readouts of lipid specimens. However, the number of lipidomics users, variety of non-standardized applications and methods is rapidly growing, risking to further extend the discrepancies in data reporting and study irreproducibility. In this lipidomics workshop, we aim to introduce the newly founded International Lipidomics Society (ILS) and discuss its role in the lipidomics and connecting communities. The workshop will be designed to introduce the ILS flagship that aims to foster international community-wide coordination and communication for the creation of lipidomics specific guidelines for good scientific practice. We will introduce the aims of the various interest groups of the society and stimulate discussion on the current and future needs. This workshop aims to explain why everyone's voice matter and encourage users to become an active part of ILS, and in this way take an active role together with the ILS community in the next developments of the lipidomics discipline. A group of experts will share their roles in ILS, aims of the working groups, and answer any questions or views from the audience.

Wed-14
Top Down Proteomics and Top Down Mass Spectrometry: Adoption and Expanding Applications
Top-Down Proteomics Interest Group

Presiders: Frederik Lermyte, Joe Cannon,

When applicable, top-down (TD) protein mass spectrometry potentially enables comprehensive characterization of proteoforms and avoids the pitfalls associated with traditional bottom-up workflows. While the TD approach is conceptually simple, technical challenges must be overcome to successfully perform a TD experiment. In this workshop, we will showcase talks from experts in both industry and academia in TD mass spectrometry and TD proteomics to propagate utilization of the technique across disciplines. The emphasis in this workshop will lie in education, practical instruction, and utilization of TD proteomics and TDMS, with the goal of constructive discussion for both novices and experts. We will discuss: characterization vs. identification and how it applies to top-down mass spectrometry; native mass spectrometry and native top-down proteomics; the application of biotransformation in protein therapeutics; and the use of top-down proteomics in biomedical research. Each topic will be introduced by a short webinar, followed by approximately 10 minutes of audience discussion and debate. Thus, a key part of the workshop will be audience participation and a lively discussion amongst attendees. Contact workshop chairs if you are interested in presenting an introduction to spark the discussion of a topic.

Thurs-01
The NIH and NSF Review and Funding Process
Special Service

Presiders: Salvatore Sechi, Douglas Sheeley, Kelsey Cook

Many ASMS members and conference participants are supported by the National Institutes of Health or 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 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.

Thurs-02
Advances in Automation for Proteomics Sample Preparation
Independent

Presiders: Michael Ford, Michael Knierman,

The performance of modern mass spectrometers and liquid chromatography systems is enabling proteomics experiments with previously unobtainable throughput and sensitivity. The analysis of cohorts of 50 or more samples, with acquisition timelines of a week or so, is now routine in many labs. Combined with robust sample preparation workflows and turnkey data processing proteomics is delivering on the promise and approaching a new level of usefulness. Assay and sample type aside it is fair to say, for proteomics experiments, the bottleneck is still instrument time. That said sample preparation is a significant use of human resources and with the scale of experiments expanding so too is the associated time and investment in labor. A practical solution to ease the growing sample preparation burden is automation. Vendors have stepped up to deliver automation solutions such as the Agilent AssayMap, ThermoFisher KingFisher and more recent low cost OpenTrons OT2. This workshop is an opportunity to get together with like-minded scientists and discuss the emerging role of automation in sample preparation for proteomics experiments and to share practical experience with automation.

Thurs-03
Cannabis & Hemp Mass Spec Workshop: A Closer Look at the Applications of Mass Spectrometry in Cannabis quality control, compliance and research
Independent

Presiders: Scott Kuzdzal, Toby Astill,

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.
Mass spectrometry is playing an increasingly important role in product quality and compliance safety testing. This testing requires accurate identification and quantification of the analytes of interest in often challenging matrices to low detection requirements (ppb). This session will review applications of MS in regulatory environments, quality control testing labs as well as emerging academic, clinical and industrial areas, including advanced agricultural, nutritional and bioscience programs. Join us as we review and discuss current and future applications of mass spectrometry in advancing cannabis/hemp science.

Thurs-04
Developing World: Supporting Education and Research in Mass Spectrometry
Independent

Presiders: Hendrik Kersten, Giles Edwards,

In 2017 Kym Faull (UCLA) initiated this workshop and has successfully organized it at the following annual ASMS meetings. The basic idea is to bring together members of our society who wish to contribute to mass spectrometry related education and research in the Developing World. At the meeting in 2019 the 25 attendees clearly stated that the goal of bringing mass spectrometry to the Developing World is an important step toward addressing the big issues mankind is facing, and will be facing in future. One central point is the transfer of discarded, but still running MS to institutions in countries that could otherwise not afford such instrumentation. However, there is a long way from goodwill to meaningful scientific data, paved with administrative, technical and educational hurdles. Sustainable development requires a profound network of experienced mass spectrometrists that provides on-site installations, trainings, potential equipment for donation and contact persons who are prepared to share knowledge, time, and expertise.
With the News and Views section in the JASMS October 2019 issue we accomplished a great step forward in broadly informing our society about the current efforts and needs, in particular about the work of RORO (Recycling Organization Research Opportunities) a registered charity organization operating in this field since 2006. To maintain the momentum and further develop this network we urgently need to meet, discuss and organize things at this year´s workshop. The agenda includes a report on the current status and capabilities of RORO and a broad discussion on our specific input.

Thurs-05
The Proteomics Standards Initiative and ProteomeXchange: Supporting open data practises in the proteomics field
Independent

Presiders: Juan Antonio Vizcaino, Eric W. Deutsch,

The Proteomics Standards Initiative (PSI, http://www.psidev.info) and ProteomeXchange (http://www.proteomexchange.org) are two highly collaborative projects that are open to the contribution and ideas from everyone in the community. Since 2002, the mission of the PSI is the development and promotion of open data standards and the related software in the proteomics field. Additionally, the PSI is increasingly involved in the development of data standards for metabolomics. 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 showcase our most successful projects and highlight some of our ongoing activities, highlighting current trends in re-use of public proteomics datasets and fostering discussion among participants about what future directions in both initiatives would most benefit the community. Please attend if you want your voice to be heard!

Thurs-06
MS-Based Process Analytical Technology (PAT): Monitoring Everything from Large Molecules to Cell Therapies
Pharmaceuticals Interest Group

Presiders: Rich Rogers, Glenn Harris,

The biotherapeutic landscape is continuously changing. The modalities used to treat patients include large molecules, small molecules, and cell and gene therapies. A significant goal of biotherapeutic process development (PD) is to produce the same high-quality product in every experiment regardless of scale. To achieve this goal, PD scientists need to employ process analytical technologies (PAT) that can provide data on the upstream process (e.g., temperature, pH, glucose, amino acids, cell viability, and metabolites), downstream process (e.g., process-related impurities and host-cell impurities) and product quality attributes of the final product (e.g., charge isoforms, aggregates, glycoforms, cell viability, and CAR frequency). Mass spectrometry (MS) is a precious tool for characterizing drug substance and drug product for every type of modality. MS is used to identify critical quality attributes that affect the safety and efficacy of the drug product. However, MS-based PAT may also be used to characterize in-process molecules and study other upstream and downstream parameters that dictate the attributes of the final drug product. This workshop will be an interactive discussion amongst a panel of experts and the workshop attendees on the current state of mass spectrometry-based PATs and how they are improving PD. Topics may include application of MS for real-time (on-line / at-line) analysis of in-process materials, automated sample handling/preparation, automated data processing, charge isoform characterization, and characterization and monitoring of cell therapy products and intermediates. Please join us to ask questions, share your knowledge and experience, and discuss the future of MS-based PAT.

Thurs-07
Career Opportunities for Chinese Students and Scholars
Independent

Presiders: Hui Zhang, Liang Li,

With the emerging development of mass spectrometry technologies and the increasing needs for applications of mass spectrometry in academic researches, 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 path after completing their training in mass spectrometry. We will invite four speakers from academia, industry, clinic, and regulatory agency 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 needed for both students and scholars of all ASMS members and potential employers and will provide opportunities for students and scholars to prepare their career development during and after mass spectrometry training and help them to make career development choices in the field of mass spectrometry

Thurs-08
Polymeric Materials Interest Group - Investigating Polymer Architecture
Polymeric Materials Interest Group

Presiders: Christina Mastromatteo, Jessica Hoskins,

This year's meeting will consist of three distinct sections; a workshop, student poster elevator-talks and an open forum.
To start with, we will have a short tutorial and updates on analysis of polymer architecture by ion mobility mass spectrometry. This topic was of great interest to the polymer community during last year's workshop.
Secondly, we will host a series of short Polymer Section poster presentations (3-5 min each) by students / presenters regarding their upcoming posters. This will provide each presenter an opportunity to promote their work externally to a professional scientific audience in their specialized field.
There will then be an open forum, in which attendees are invited to bring up any polymer-related issues or questions that they would like help with. In addition, input will be sought for future Polymer Workshop topics.

Thurs-09
Ambient Ionization: How can we make it more reproducible?
Independent

Presiders: G. Asher Newsome, ,

Dozens of ambient ionization sources for mass spectrometry have been created since the introduction of desorption electrospray ionization (DESI) and direct analysis in real time (DART) in the mid-2000s. These ambient ionization tools are capable of direct examination of samples in real-time with minimal-to-no sample preparation. In last year's workshop, reproducibility was flagged as one of the main concerns that slows the adoption of ambient ionization. This year we will have brief expert presentations on improving the reproducibility of ambient ionization sources springboarding a more extended discussion on strategies for improvement and possible trade-offs. The ambient ionization workshop aims to encourage the participation and presentations of new investigators, postdocs, and graduate students with a balanced perspective from academia, non-academic labs, and industry. One of the goals of the workshop will be to gather scientists interested in ambient ionization technology and discuss the formation of an ambient ionization interest group to address these new scientific challenges.

Thurs-11
Machine learning analysis of mass spectrometry data in the life sciences
Bioinformatics MS Interest Group

Presiders: William Noble, Arzu Guler,

The field of machine learning involves applying a variety of statistical models to big, heterogeneous data sets. To an increasing degree, machine learning technology is at work in many places -- our phones, our music players, our web browsers. On the other hand, although some types of mass spectrometry analysis already use machine learning tools to help make sense of large collections of spectra, we believe that the mass spectrometry community is currently under-utilizing machine learning techniques. Accordingly, this workshop will focus on success stories of applying machine learning to the analysis of proteomics data in the life sciences, and on exploring possible future directions where learning methods could be of particular value. We will emphasize the breadth of types of problems that can be solved using machine learning techniques, going beyond the standard tasks of classification and regression. Several case studies will demonstrate concrete applications, emphasizing their reasons for success. Our goal will be two-fold: to spur workshop attendees to brainstorm potential applications of machine learning to problems that they want to solve, and to teach attendees how to recognize what makes a problem well-suited (or not) to a machine learning approach.

Thurs-12
Standardizing the Imaging MS Workflow: Current Progress
Imaging MS Interest Group

Presiders: Peggi Angel, Tiffany Porta,

Progress continues to be made in standardizing imaging mass spectrometry workflows and the current imaging MS work has advanced to include studies of large interlaboratory comparisons for clinically applied workflows. From these investigations, a number of new tools and strategies have emerged for reproducibly transferring workflows between laboratories. In this workshop, we will discuss the state of the art for reproducibly transferring Imaging MS workflows between laboratories. Preliminary topics to be addressed include:
1)   Challenges and solutions for instrument specific method transfer
2)   Standardization tools from reference tissues to applied internal standards
3)   Tools & strategies for sharing and comparing data
4)   Minimum requirement and documentation of guidelines for successful method transfer
The workshop will entail short presentations by students, postdoctoral fellows, investigators from industry, academia, and government laboratories. Each presentation will be followed by a 5-10 minutes discussion within the interest group. A goal is to further disseminate information on challenges and solutions for method transfer between laboratories.

Thurs-13
Leveraging Emotional Intelligence Strategies during the Pandemic
Career Development Interest Group

Presiders: Lucinda Hittle, Charles Veltri,

The CoVID-19 global pandemic has brought to the forefront of our existence mindfulness and managing our ability to handle stress, uncertainty and chaos. Intentional application of emotional intelligence strategies can help everyone work through these challenging times. This workshop will convene scientists across diverse sectors including academia, industry, government and non-profit agencies. The panel will discuss coping strategies during the global pandemic leveraging the four elements of emotional intelligence: self-awareness, self-management, social awareness and relationship management. Time will be provided for audience participation through Q&A and discussion. The goals of this interest group continue to be to foster relationships across the society that span the boundaries of geography, age, level of experience, and academic training as well as enabling networking and small group discussions. Let's get through this together!

Thurs-14
The Multidimensional Clinical Space - From Discovery to Practice in Screening and Diagnostics
Clinical Chemistry Interest Group

Presiders: Candice Ulmer, Don Chace,

Clinical laboratory measurements for both screening and diagnostics require the implementation of quality control and quality assurance (QA/QC) procedures to ensure accuracy/reliability in laboratory measurements, consistent disease diagnosis, and appropriate treatment for patients. However, there is a need to identify and harmonize these QC/QC procedures across multiple analytical platforms for applications involving screening and diagnostics. This workshop will highlight best practice QC/QA standards that can be applied in targeted and multi-analyte assays across multiple applications and mass spectrometric platforms. Representatives from industry, regulatory bodies, and clinical hospital laboratories will deliver brief presentations on their considerations of the proposed QA/QC measures, followed by an open forum in which the expectations for the implementation of these QA/QC best practices will be discussed.

Thurs-15
Large-Scale Data Analysis and Management: Challenges for Analytical Laboratories
Analytical Lab Managers Interest Group

Presiders: Samuel Mackintosh, Ryan Leib,

Data analysis and management continue to present significant challenges for analytical laboratories that generate large data sets. Two major factors complicating the development of broadly applicable solutions to these challenges are (1) the rapid advance of technological capabilities and analytical methods in the field of mass spectrometry, and (2) the need to prepare and deliver data for further interpretation and publication by principal investigators who are not mass spectrometrists or bioinformaticists. With these challenges in mind, the 2020 ASMS Analytical Lab Managers Workshop will focus on techniques for processing and management of data from emerging methodologies in ways that meet the needs of non-specialist clients and collaborators. The workshop will feature three speakers discussing the analysis and management of different types of data, followed by a group discussion period.

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