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**MP 001**
A Real Time Metabolomic Profiling Approach to Authentication of Ginkgo Biloba Extracts Products Using Rapid Evaporative Ionization Mass Spectrometry; Yisheng Xu1; 2; Jinghui Wang1; 3; Shuang Fang1; 2; Kate Yu2; Jihong Lin2; Hongzhu Guo3; Zhongshi Qian1; 1Chinese Pharmacopeia/Waters Joint Open Lab, Beijing, China; 2Waters cooperation, Shanghai, China; 3Beijing 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 Zaitsu1; 2; Seiichiro Eguchi3; Tomomi Ohara4; Akira Ishii5; Takakazu Kawamata6; Akira Iguchi7; 1In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; 2Nagoya University Graduate School of Medicine, Nagoya, Japan; 3Department of Neurosurgery, Tokyo Women’s Medical University, Tokyo, Japan; 4Marine 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 QToF system; Vishal Mahale1; Dipankar Malakar2; Rashid Faraz3; Dharmeshkumar Parmar4; 5; Subodh Chawan6; Venkateswarlu Panchagnula1; 2; 3; 4; Barfeet Analytics Pvt. Ltd., Pune, India; 2AB Scix, India, Gurgaon, India; 3AB Sciex, India, Gurgaon, India; 4CSIR-National Chemical Laboratory, Pune, India, Pune, India; 5Academy of Scientific and Innovative Research (AcSIR), Pune, India; 6Scientia Life Technologies LLP, Mumbai, India

**MP 004**
Rapid Flux Phenotyping by DESI-Ion Mobility-Imaging Mass Spectrometry to Accelerate Metabolic Engineering of Bacteria; Berkley Ellis1; 2; Piyosh Babel1; Jody C. May2; Brian Pfleger3; Jamey Young4; John A. McLean5; 1Vanderbilt University, Nashville, TN; 2Vanderbilt University, Nashville, TN; 3University of Wisconsin, Madison, WI

**MP 005**
Versatile (applications with) metalspray in mass spectrometry using hydrophobic/omniohobic surfaces; Michael C Godwin1; William Hoffmann1; 1Texas State University, San Marcos, TX

**MP 006**
Python-powered kinetic analysis of data rich mass spectrometric reaction monitoring; Sofia Donnete1; Brett Henderson2; Scott Mcindoe2; 1University of Victoria, Victoria, BC; 2University of Victoria, Victoria, British Columbia

**MP 007**
Analysis of Cholesterol and Androgens in Mouse Prostate Cells by LC-MS/MS: HESI versus APCI; Min Liu1; Jayden K. Cline1; Asmaa Elkenawi1; Brian Ruffell1; John M. Koomen1; 1Moffitt 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 Stevens1; German Augusto Gomez-Rios1; Gary Stidsen1; David S. Bell1; 1Barefeet Analytics Pvt. Ltd., Pune, India; 2AB Sciex, India, Gurgaon, India; 3AB Sciex, India, Gurgaon, India

**MP 010**
Software tool for visual inspection of the stability and reproducibility of mass spectra; Evgeny Zhvansky1; Anatoly Sorokin1; Daniil Ivanov1; Denis Zavorotnyuk2; Stanislav Pekov1; Vasily Eliferov1; Eugene (evgeny) Nikolaev2; Igor Popov3; 1Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 2Skolkovo 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 Khaled1; Janusz Pawliszyn1; 1University of Waterloo, Waterloo, ON

**MP 012**
High-throughput Determination of Pesticides using DART-QTOF MS; Wei Du1; Wei Chen2; Kerry Song3; Xiaokun Duan2; 1Agilent Technologies, Beijing, China; 2ASPEC Technologies, Beijing, China

**MP 013**
Reactive Flowing Atmospheric Pressure Afterglow for Derivatization Analytes in Real-time.; Dong Zhang1; Maureen Oliva1; Gerardo Gamez1; 1Texas Tech University, Lubbock, Texas

**MP 014**
Modified Conical Ablation Chamber for Remote Laser Ablation Electrospray Ionization Mass Spectrometry; Marjan Dolatmoradi1; Jarod A. Fincher2; Andrew R. Korte3; Nicholas J. Morris2; Akos Vertes1; 1The George Washington University, Washington, DC; 2Air 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 Bensussan1; Tanweer Zaidi2; Ruth Katz2; Livia S. Eberlin1; 1The University of Texas at Austin, Austin, TX; 2MD Anderson, Houston, TX

**MP 016**
Solid Phase Microextraction Probe Electrospray Ionization for Quantitation of Drugs of Abuse in Small Volumes of Plasma; Milana Thirukumar1; Varoon Singh1; Yohei Arao2; Yuka Fujito2; Masayuki Nishimura3; Hidekazu Saiki2; Yoshihiro Hayakawa3; Janusz Pawliszyn1; 1University of Waterloo, Waterloo, ON; 2Shimadzu Scientific Instruments, Inc., Columbia, MD; 3Shimadzu Corporation, Kyoto, Japan
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MP 017  Capturing Fleeting Intermediates in Uncatalyzed Claisen Rearrangement under Non-Equilibrium Droplet Imbibition Conditions; Taghi Sahraei1,2; Abraham K. Badu-Tawiah1; 1The Ohio State University, Columbus, OH

MP 018  Dual desorption electrospray ionization and laser mass spectrometry imaging using the same interface; Lauren H Katz1; Michael Woolman1; Francis Talbot1; Siham Amara-Belgadi2; Megan Wu2; Sara Tortorella3; Sunit Das4; Howard Ginsberg4; Arash Zarrine-Afsar1; 1University of Toronto, Toronto, Ontario; 2Peter Gilgan Centre for Research and Learning, Hospital for Sick Children, Toronto, Ontario; 3Molecular Horizon, Bettona, Italy; 4St. Michael's Hospital, Toronto, Ontario

MP 019  Studies of reaction acceleration in microdroplets, thin films and sealed microchannels; Lingqi Qiu1; Zhenwei Wei1; Honggang Nie1,2; R. Graham Cooks1; 1Purdue University, West Lafayette, IN; 2Peking University, Haidian, China

MP 020  Serine Enhances Protein Analysis by DESI-MS; Roshan Javanshad1; Andre R Venter1; 1Western Michigan University, Kalamazoo, MI

MP 021  High-yield gram-scale organic synthesis using solvent recycling accelerated microdroplet/thin film reactor; Honggang Nie1,2; Zhenwei Wei1; Lingqi Qiu1; Xingshuo Chen1; Dylan T. Holden1; R. Graham Cooks1; 1Purdue University, West Lafayette, IN; 2Peking University, College of Chemistry, Beijing, China

MP 022  Monitoring peppermint washout in the breath metabolome by secondary electrospray ionization-high resolution mass spectrometry; Jiayi Lan1; Renato Zenobi1; 1ETH 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 Birse1; Olivier Chevallier2; Sara Stead3; Steven Pringle4; Vil Kosek4; Vojtech Hrebek4; Jana Hajsova4; Christopher Elliot5; 1Institute for Global Food Security, Queen’s University Belfast, Belfast, United Kingdom; 2Mass Spectrometry Core Technology Unit, Queen’s University Belfast, Belfast, United Kingdom; 3Waters Corporation, Wilmslow, United Kingdom; 4University of Chemistry and Technology, Prague, Czech Republic

MP 024  Reaction Acceleration at Air-Solution Interfaces: Anisotropic Rate Constants for Katritzky Transamination; Yangjie Li1; Tsdale F. Mehari1; Zhenwei Wei1; Yong Liu2; R. Graham Cooks1; 1Purdue University, Lafayette, IN; 2Merck & Co., Rahway, NJ

MP 025  Rapid Quantitative Screening of Cyanobacteria for Anatoxins Using Direct Analysis in Real Time-High Resolution Mass Spectrometry; Daniel Beach1; Cheryl Rafuse1; Jeremy E. Melanson2; Pearse Mccarron1; 1Biotoxin Metrology, National Research Council Canada, Halifax, NS; 2Organic Chemical Metrology, National Research Council Canada, Halifax, NS

MP 026  Analysis of Oceanic Systems by TM-DART-QTOF-MS-Based Seaomics; Nicolas Zabalegui1; Malena Manzi1; Antoine Depoorter2; Nathalie Hayeck3; Marie Roveretto2; Chunlin Li2,3; Manuela Van Pinxteren4; Hermann Hartmut5; Christian George6; Maria Eugenia Monge1; 1Centro de Investigaciones en Bionanociencias (CIBION), CONICET, Buenos Aires, Argentina; 2Université de Lyon 1, CNRS, IRCELYON, Villeurbanne, France; 3Weizmann Institute of Science, Rehovot, Israel; 4Leibniz-Institut für Troposphärenforschung e.V., Leipzig, Germany

MP 027  In vivo mapping of cell type-specific interactome study in mouse brain; Xiaojun Sun1; Xian Han1; Huan Sun2; Ping-Chung Chen1; Yun Jiao1; Junmin Peng1; 1St jude Children’s research hospital, Memphis, TN; 2St. 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. Wellgamage De Silva1; Thomas D Kisela1; Alleigh Nicole Couch1; Cristina Castillo1; Guido F. Verbeck1; 1University 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 Ramonaitė1; Alvaro Perdones-Montero1; Andrew Ray1; Miriam Guest1; Simon Cameron1; Zoltan Takats1; 1Imperial College London, London, United Kingdom; 2AstraZeneca, Macclesfield, United Kingdom

MP 030  Programmed Droplet Desolvation And Occam's Razor; Drew Sauter1; Andrew D Sauter III1; Ron Shomo2; 1Nanoliter, LLC, Henderson, NV; 2Adaplas, Palmer, MA, Massachusetts

MP 031  Non-proximate Ambient Sampling for Solvent-free Analysis of Intact Objects; G. Asher Newsome1; Kathleen Martin1; Julia Campbell-Such2; 1Smithsonian Museum Conservation Institute, Suitland, MD; 2Smithsonian National Museum of the American Indian, Hillcrest Hills, MD; 3Smithsonian National Museum of African Art, Washington, DC

MP 032  Counterions for Ambient Ion Focusing; Saquib Rahman1; Brett M. Marsh1; Shane Tichy2; R. Graham Cooks1; 1Purdue University, West Lafayette, IN; 2Agilent Technologies, Santa Clara, CA
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MP 033 Condensed Liquid Aerosol Particle Spray (CLAPS) Coupled to MS – a Novel On-Line Liquid Aerosol Analysis Technique; Nathanael A Park1; Spencer E Tilley1; Gary L Glish1; 1UNC Chapel Hill, Chapel Hill, NC

MP 034 Quantitation with Direct Analysis in Real Time Mass Spectrometry by utilizing less sample; Paul Liang1; Frederick Li1; Brittany Laramee1; Brian Musselman1; 1IonSense,Inc., Saugus, MA

MP 035 An Integrated Microfluidic probe for High-Resolution and High-throughput Nano-DESI Mass Spectrometry Imaging of Tissue Sections; Xiangtang Li1; Ruichuan Yin1; Julia Laskin1; 1Purdue University, West Lafayette

MP 036 Serine sublimation: from racemic crystal to homochiral octamer in gas phase; Rong Chen1; Zhenwei Wei1; R. Graham Cooks1; 1Purdue University, West Lafayette, IN

MP 037 Combined Mechanospray Ionization with a Discharge Needle Shifts Charge State Distributions in Real-Time; Liam Dugan1; Mark E Bier1; 1Carnegie 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; Vilmos Kertesz1; John F. Cahill1; Scott T. Retterer1; Muneeba Khalid1; Courtney L. Walton1; 1Oak Ridge National Laboratory, Oak Ridge, TN

MP 039 Novel Systems and Methods for Picoflow Electrospray; Mengtian Li1; Linfan Li2; Jae Schwartz2; Anyin Li1; 1University of New Hampshire, Durham, NH; 2Thermo Fisher Scientific, San Jose, CA

MP 040 Investigating Molecular Extraction and Ionization Processes in Solvent-Based Ambient Ionization Mass Spectrometry; Monica Lin1; Molly S. Blevins1; Marta Sans1; Jennifer S. Brodbelt1; Livia S. Eberlin1; 1University 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; Thomas P. Forbes1; Edward Sisco1; Matthew Staymates1; 1National Institute of Standards and Technology, Gaithersburg, MD

MP 042 Integration of 3D Printing into Desorption Electrospray Ionization Mass Spectrometry; Kevin J Zemaitis1; Kathiravan Kaliyappan1; Vp Krishnan Muthaiah1; Alexis C Thompson1; Troy D Wood1; 1University of Buffalo, Buffalo, NY

MP 043 Cone-jet mode electrospray ionization in microflow and nanoflow regimes by emitter surface manipulations; Sau Lan Staats1; Anna Stoltzfus1; Andris Suna1; 1Phoenix 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; German Augusto Gómez-Ríos1; Shane Stevens1; David S. Bell1; Gary Stidksen1; 1Restek Corporation, Bellefonte, PA

MP 045 Nanometer Scale Chemical and Functionalons Imaging on an AFM-MS System; Ryan Wagner1; Matthias Lorenz2; Olga S. Ovchinnikova1; Roger Proksch1; 1Oxford Instruments, Goleta, CA; 2University of Tennessee Knoxville, Knoxville, TN; 3Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

MP 046 Implementation of marker tips for touch spray ionization; Roman Levin1; Denis Bormotov1, 2; Konstantin Bocharov1, 2; Anna Mishina1; Vsevolod Shurkhay1; Stanislav Pekov1, 2; Eugene (evgeny) Nikolaev1; Igor Popov1; 1Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 2V.L. Talrose Institute for Energy Problems of Chemical Physics, N.N. Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; 3Skolkovo institute of science and technology, Moscow Region, Russian Federation

MP 047 Application of a non-fixed magnetic carbon nanotube paper in paper spray analysis; Tâssia Venga Mendes Venga Mendes1; Eduardo Costa De Figueiredo2; Nicholas E. Manicke1; 1Indiana University Purdue University Indianapolis, Indianapolis, IN; 2Federal University of Alfenas, Alfenas, Brazil

ANTIBODIES & ANTIBODY DRUG CONJUGATES I

MP 048 Site specific glycan profiling of N-glycans from Cetuximab; Min Kyung So1; Chung Su Lim1; Ju Hyeon Lim1; In Young Ko1; Ah Young Ki1; Byoung Joon Ko1; 1Kbiohealth, Cheonju-si, South Korea

MP 049 Distinguishing of isomeric Leu/Ile residues by Integrated LC-hot ECD MS/MS in an RF Ion Trap; Khadijeh Rajabi1; Takashi Baba1; 1SCIEX, Concord, ON

MP 050 Study of glycosylation in Monoclonal Antibody using Intact and Middle-Down Approach; Kejin Chen1; Takashi Baba1; 1SCIEX, 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; Hanna Toffevel1; Philip J. Widdowson1; Andreas Nägeli1; Helen Nyhlin1; Fredrik Olsson1; 1Genovis AB, Lund, Sweden; 2Thermo Fisher Scientific, Runcorn, United Kingdom

MP 052 Offline IEX fractionation of monoclonal antibodies enhances coverage of proteoforms in native CZE-MS analysis; Kendall Johnson1; Erica Teng1; Marcia Santos2; Alexander R. Ivanov1; 1Northeastern University, Boston, MA; 2Sciex, Brea, CA
**MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.**

**MP 053** Comprehensive Characterization of Monoclonal Antibody and Antibody Drug Conjugate on a Hybrid Quadrupole-Orbitrap Mass Spectrometer; Kristina Srzentic1; Eugen Damoc2; Angela Criscuolo3; Tom Buchanan4; Kristina Radi5; Marc Guender6; 1Thermo Fisher Scientific, Cambridge, MA; 2Thermo Fisher Scientific, Bremen, Germany; 3Thermo Fisher Scientific, Dreieich, Germany; 4Thermo Fisher Scientific, Runcorn, United Kingdom; 5Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; 6Thermo Fisher Scientific, reinach, Switzerland

**MP 055** Characterization of O-glycosylation by mass spectrometry to support process development of an Fc-fusion protein; Renpeng Liu1; Rachel Chen2; Zoran Sosic3; 1Biogen, Cambridge, MA

**MP 056** Characterization and comparison of Neulasta and its biosimilar at intact level on a quadrupole-Orbitrap mass spectrometer; Xiaoxi Zhang1; Haichuan Liu2; Hao Yang3; Min Du4; 1ThermoFisher Scientific, Shanghai, China; 2Thermo Fisher Scientific, San Jose, California; 3ThermoFisher Scientific, Massachusetts, Massachusetts

**MP 057** TSPR-MS: New Online Epitope Analyzer for Epitope and Affinity Determination of Antibody-Ligand Interactions; Frederik Barka1; Loredana Lupu2; Pascal Wiegand2; Delia Miho2; Oliver Mueller2; Friedemann Voelklein3; Guenes Barka4; Michael Przybylski5; 1Sunchrom GmbH, Friedrichsdorf, Germany; 2Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spec, Ruesselsheim, Germany; 3Rhein 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 Cutak1; Ken Chanthamontri2; Kevin Ray3; 1MilliporeSigma, St. Louis, MO

**MP 059** Linking Biochemical and Biophysical Antibody Drug Conjugate (ADC) Data in Assessing Drug-to-Antibody Ratio (DAR); Colette Quinn1; Henry Shion2; 1Waters Corporation, Milford, Massachusetts; 2Waters Technologies Corporation, Milford, MA

**MP 060** Rapid microfluidic molecular weight determination and spent media analysis for an IgG1 intact protein in growth media; Adi M Kulkarni1; Kenion H Blakeman2; Kathryn Elliott3; Colin M Gavin4; Yi Young L Anderson5; Sarah Harcum6; Glenn A Harris7; 1908 Devices, Inc., Boston, MA; 2Clemson 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 Niu1; Daniel Ladrör2; Gary Jenkins3; John Paul Savaryn4; 1Abb Vie Inc, North Chicago, IL

**MP 062** Combination of Hybrid LC-MS and HR-MS Techniques to Characterize Uncialamycin Antibody Drug Conjugates; Jose Trinidad1; Amanda Valdiosera1; Hetal Sarvaiya1; Christine Gu2; Julia Gavriluyk3; Beth Pysz4; 1Abbvie 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 Zhang1; Tom Ding1; Samir Das2; Andrea Hernandez3; Jodi Wong4; Dunja Urosev5; Jamie Rich6; 1Zymeworks Inc., Vancouver, BC

**MP 064** TArget-Responsive SubCellular Pharmacokinetics for Early-stage Antibody-Drug Conjugates Screening and Assessment; Jiali Liu1; Hua Sang2; Xiaofang Zhang3; Ning Wang1; Yanzhou Liu1; Guangj Wang1; Hui Ye1; 1China Pharmaceutical University, Nanjing, China; 2Department of Pharmacy, The Affiliated Hospital of Nantong University, Nantong, China

**MP 065** Discovery of photoinduced cross-links in monoclonal antibodies; Thomas Powell1; Michael Knight1; John O’Harra2; William Burkitt3; 1UCB, Slough, United Kingdom

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**CANNABIS**

**MP 066** Analysis of Tetrahydrocannabinol Vape Oils Using Pyrolyzer; Karen Sam1; Ben Landas1; 1CDS Analytical, Oxford, PA

**MP 067** MALDI-MS Library of Fingerprint Spectra for Selected Fractions of Cannabis Products; Baylie Gigolyk1; Helene Perreault1; 1University of Manitoba, Winnipeg, MB

**MP 068** Methodology for Targeted and Non-Targeted Screening and Differentiation of Cannabis Cultivars; Marian Twohig1; Steven Lai2; Angus Black2; Christopher Hudalla3; Justin Chang1; Kenneth Rosnack2; 1Waters Corporation, Milford, MA; 2Nonlinear Dynamics, Newcastle upon Tyne, United Kingdom; 3Proverde 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 Alonso1; Elizabeth Humston-Fulmer1; Christina Kelly1; Joe Binkley1; 1Leco Corporation, St. Joseph, MI
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

MP 070  Detection of typical GCMS Pesticides in Cannabis Matrix utilizing APCI-LCMS; Jennifer C Davis¹; Evelyn H Wang²; Katie Pryor²; Priyanka Chitranshi²; Christopher T. Gilles²; ¹Shimadzu Scientific Inc., Columbia, MD; ²Shimadzu 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); Stephan Altmaier; Merck KGaA, Darmstadt, Germany

MP 072  Method development for pesticides analysis in cannabis oil; Xuejun Zang¹; Asha A. Oroskar¹; Anil Oroskar¹; ¹Orochem Technologies Inc Naperville, IL

MP 073  An in-depth evaluation of accuracy in cannabis potency testing methods; Zachary Kelley¹; Bert C. Lynn¹; ¹Department of Chemistry, University of Kentucky, Lexington, KY

MP 074  Developing a discovery-based approach to cannabis testing using GC×GC-TOF MS; Laura McGregor¹; Bob Green¹; Matthew Edwards²; David Bowman³; Wade Bontempo³; Kevin Kyle³; ¹SepSolve Analytical, Peterborough, United Kingdom; ²SepSolve Analytical, Waterloo, ON; ³Markes International Inc, Sacramento, CA

MP 075  QUALITATIVE/ QUANTITATIVE ANALYSIS OF A METABOLIC PATHWAY IN POPULAR CBD BEVERAGES & OILS USING GC-MS & UHPLC-HRMS; Eloisa Franco¹; Vedanga Arekar¹; Maria Alejo-Diaz¹; Sneha Kadam¹; Dil Ramanathan¹; ¹Kean University, Union, NJ

MP 076  Comparative Analysis of Kava and Industrial Hemp Using GC-MS; Dhara Patel¹; Daniel George²; Sneha Kadam¹; Eloisa Franco¹; Yuriko Root¹; Dil Ramanathan¹; ¹Kean University, Union, NJ; ²Ridge 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; Avinash Dalmia¹; Saba Hariri¹; Jacob Jalali¹; Feng Qin¹; Thomas White⁴; ¹Perkinelmer, Shelton, CT; ²Perkin Elmer, Wood bridge, ON; ³PerkinElmer, Inc., San Jose, CA; ⁴PerkinElmer, Shelton, CT

MP 078  A Fast, Sensitive and Comprehensive Assay to Quantify 16 Cannabinoids in Hemp Plant using LC/MS/MS; Aihua Liu¹; Daniel Taylor¹; Amy Wei¹; Spencer Carter¹; ¹Dyad Labs, Salt Lake City, UT

MP 079  Analysis of the California list of pesticides and mycotoxins in cannabis edibles; Nathaly Reyes Garces¹; Colton Myers¹; Ashlee Gerardi¹; ¹Restek Corporation, Bellefonte, PA

MP 080  Future-proofing Cannabis analysis with a hybrid triple quadrupole/linear ion trap system; Katherine Hyland¹; Robert Di Lorenzo¹, ²; ¹SCIEX, Redwood City, CA; ²SCIEX, Concord, ontario

MP 081  Analytical Workflows Using Orbitrap Mass Spectrometry to Evaluate Potency in Cannabis-Containing Edibles; Ryan Hayward¹; Rob O'brien¹, ²; Matthew Noestheden¹, ²; ¹Supra R&D, Kelowna, BC; ²University of British Columbia, Kelowna, BC

MP 082  Development of a Robust LC-MS/MS Method for the Simultaneous Quantification of Cannabidiol (CBD), Tetrahydrocannabinol (THC) and their Metabolites in Plasma; Mays Al-Dulaymi¹; Christine Allen¹; ¹Leslie Dan Faculty of Pharmacy, University of Toronto, Toronto, ON

CARBOHYDRATES I

MP 084  Structural determination of polysaccharides using logically derived sequence tandem mass spectrometry; Chi-Kung Ni; ¹Academia Sinica, Taipei, Taiwan

MP 085  Sialylation Status and Mechanical Properties of THP-1 Macrophages Upon LPS Stimulation; Yu Zhao¹; Gautam Mahajan¹; Chandrasekhar Kothapalli¹; Xue-Long Sun¹; ¹Cleveland State University, Cleveland, OH

MP 086  Monitoring Oligosaccharides From Glycosyltransferase Reactions Using Paper Spray Mass Spectrometry (PS-MS); Qi Wang¹; Pengyi Zhao¹; Matrika Bhattarai¹; Michael Held²; Ahmed Faik²; Hao Chen¹; ¹New Jersey Institute of Technology, Newark, NJ; ²Ohio 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; Neil Gregory Rumachik; Thermo Fisher Scientific, Sunnyvale, CA

MP 088  Structural Characterization of Glycans by Electron-Transfer/Higher-Energy Collision Dissociation; Tengfei Yuan¹, ²; Juan Wei¹; Yang Tang¹, ³; Catherine E Costello¹, ³; Cheng Lin¹; ¹Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; ²Department of Clinical Laboratory, Renmin Hospital of Wuhan University, Wuhan, China; ³Department of Chemistry, Boston University, Boston, MA

MP 089  N-glycan profiling of kidney brush border membrane from rats using LC-MS/MS analysis; Ailing Yu¹; Jingfu Zhao¹; Bruce A. Moltoros²; Mark C. Wagner²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²Indiana University, Indianapolis, IN
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

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

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

MP 092  Negative Ion Mode Electron Capture Dissociation of Synthetic Heparan Sulfate Oligosaccharides; Isaac Agyekum; Adrian Kim; Lauren Pepi; Jonathan I Amster; 1University of North Georgia - Gainesville Campus, Oakwood GA, Georgia; 2University 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; Lauren E. Pepi; Pradeep Chopra; Geert-Jan Boons; Jon Amster; 1University of Georgia, Athens, GA

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

MP 095  Study of cnidarian-dinoflagellate symbiosis by analysis of cell surface N-glycans in dinoflagellate symbionts; Xue Dong; Wenjing Peng; Trevor R. Tivey; John Everett Parkinson; Paige E. Mandelare; Donovon A. Adpressa; Virginia M. Weis; Sandra Loesgen; Yehia Mechref; 1Texas Tech University, Lubbock, TX; 2Oregon State University, Corvallis, OR; 3University of South Florida, Tampa, FL; 4University 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; Hendrik Eshuis; 1Montclair 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; Mathieu Fanuel; Manuel Liebeke; Jan-Hendrik Hehemann; Hélène Rogniaux; Glen P. Jackson; David Ropartz; 1Max-Planck-Institute for marine microbiology, Bremen, Germany; 2Marum Center for Marine Environmental Sciences, Bremen, Germany; 3INRAE, BIBS facility, Nantes, France; 4West 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; Zachary J. Sasiene; David Ropartz; Hélène Rogniaux; Glen P. Jackson; Robert P Pellegrinelli; Thomas R. Rizzo; 1EPFL/LCPM, Lausanne, Switzerland

MP 099  Combining cryogenic infrared spectroscopy with selective enzymatic cleavage for determining glycan primary structure; Irina Dyukova; Eduardo Carrascosa; Robert P Pellegrinelli; Thomas R. Rizzo; 1EPFL/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; Vasyly Yatsyna; Priyanka Bansal; Ali H Abikhodr; Thomas R. Rizzo; 1EPFL/LCPM, Lausanne, Switzerland

CORPORATE POSTERS I

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  The development of curved LC gradient method for 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; Hady Razak Hady; Lukasz Szczersinski; Agnieszka U. Blachnio-Zabielska; Adam Kretowski; Tomasz Kowalczyk; Piotr Zabielski; 1Department of Medical Biology, Medical University of Bialystok, Bialystok, Poland; 21st Clinical Department of General and Endocrine Surgery, Medical University of Bialystok, Bialystok, Poland; 3Clinical Research Center, Medical University of Bialystok, Bialystok, Poland; 4Department of Hygiene, Epidemiology and Metabolic Disorders, Medical University of Bialystok, Bialystok, Poland
MP 106  A Novel, Q-ToF Data Independent Acquisition Method Using an RF Only Quadrupole with Scanning Dipolar Excitation; Keith Richardson\textsuperscript{1}; Martin Green\textsuperscript{1}; Chris Hughes\textsuperscript{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; Dany Jeanne Dit Fouque\textsuperscript{1}; Alicia Maroto\textsuperscript{1}; Rémy Lartia\textsuperscript{2}; Antony Memboeuf\textsuperscript{1}; CEMCA, Université de Brest, CNRS, Brest, France; UMR CNRS 5250, ICMG FR-2607, Université Grenoble-Alpes, Grenoble, France
DATA-DEPENDENT ACQUISITION

MP 108  Label-free single cell proteomics; Hila Wolf-Levy1; Tom Fleischer1; Liran Shlush1; Yishai Levin1; 1Weizmann Institute of Science, Rehovot, Israel

MP 110  Boosting DDA acquisition rates via off-instrument 3-D feature detection; Mathew Guiterrez1, 2; Rob Smith1, 2; 1Prime Labs, Inc., Missoula, MT; 2University of Montana, Missoula, MT

MP 111  Adding an MS2-based filter prior to scoring to improve the speed of multiple modification searches in SpectroMine; Lynn Verbeke1; Oliver M. Bernhardt1; Jan Muntel1; Lukas Reiter1; 1Biognosys AG, Schlieren, Switzerland

MP 112  Developments in Real-Time Search on an Orbitrap Tribrid mass spectrometer; Jesse D. Canterbury1; Graeme Mcalister1; William D. Barshop1; Tony Zhao1; Aaron M Robitaille1; Romain Huguet1; 1Thermo Fisher Scientific, San Jose, California

DATA-INDEPENDENT ACQUISITION

MP 113  Leveraging Infrared Multiphoton Dissociation for Selective Data Independent Acquisition; Joshua P. Salem1; Kristina Håkansson1; Nicholas Borotto2; 1University of Michigan, Ann Arbor, MI; 2University of Nevada, Reno, NV

MP 114  Hybrid spectral library combining DIA-MS data and a targeted virtual library substantially deepens the proteome coverage; Ronghui Lou1; Pan Tang1; Kang Ding1; Wenging Shui2; 1ShanghaiTech University, Shanghai, China; 2Human Institute, ShanghaiTech University, Shanghai, China

MP 115  High-precision ion mobility calibration greatly improves diaPASEF analysis; Tejas Gandhi1; Stephanie Kaspar-Schoenefeld2; Oliver M. Bernhardt1; David Schlessinger1; Sven Brehmer1; Gary Kruppa2; Jan Muntel1; Lynn Verbeke1; Lukas Reiter1; 1Biognosys, Schlieren, Switzerland; 2Bruker Daltonics, Bremen, Germany

MP 116  Using microflow LC-SWATH-MS with extensive peptide fractionation to interrogate the proteome of KRas-mutant cancer cells; César Alain Aguilar-Velás1; Juan F. Martinez-Aguilar2; 1Escuela Nacional de Ciencias Biológicas, Instituto Politécnico Nacional, Miguel Hidalgo, Mexico; 2Red 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; Yonghai Lu1; Zhaooqi Zhan2; 1Shimadzu (Asia Pacific) PTE LTD, Singapore, Singapore; 2Shimadzu (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 Meier1; Stephanie Kaspar-Schoenefeld2; Andreas-David Brunner1; Max Frank2; Annie Ha2; Isabell Bludau2; Eugenia Voytik1; Markus Lubeck2; Oliver Raether2; Ruedi Aebersold3, 6; Ben C. Collins4; Hannes L. Röst3; Matthias Mann1, 7; 1Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; 2Bruker Daltonik, Bremen, Germany; 3Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; 4Bruker Daltonik GmbH, Bremen, Germany; 5Department of Biology, Institute of Molecular Systems Biology, ETH Zürich, Zurich, Switzerland; 6Faculty of Science, University of Zürich, Zurich, Switzerland; 7NFF Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

MP 119  Deep Quantitative Phosphoproteomics by Data Independent Acquisition Mass Spectrometry; Reta Birhanu Kitata1; Chia-Feng Tsai2; Wai-Kok Choong2; Pei-Yi Lin1; Yun-Chien Chang1; Bo-Shiu Chen1; Alexey I. Nesvizhskii1; Ting-Yi Sung5; Yu-Ju Chen4, 6; 1Institute of Chemistry, Academia Sinica, Taipei, Taiwan; 2Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington; 3Institute of Information Science, Academia Sinica, Taipei, Taiwan; 4Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, Michigan; 5Institute of Information Science, Academia Sinica, Taipei, Taiwan; 6Department 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 Willems1, 2; Simon Daled1, 2; Bart Van Puyvelde1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Thermo Fisher Scientific, San Jose, California

MP 121  Data dependent-independence acquisition (DDIA): fusion of bottom-up proteomics paradigms in a single LC-MS/MS experiment; Shenheng Guan1, 2; Paul P. Taylor3; Ziwei Han1; Michael F. Moran4; Bin Ma1; 1University of Waterloo, Waterloo, ON; 2Hospital for Sick Children, Toronto, Ontario; 3Rapid Novor Inc, Waterloo, Ontario; 4University of Toronto, Toronto, Ontario

MP 122  High throughput proteomics - Application of diaPASEF for short gradients; Stephanie Kaspar-Schoenefeld1; Markus Lubeck1; Scarlet Koch2; Oliver Raether1; Gary Kruppa2; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker Daltonik GmbH, Bremen, Germany

MP 123  Mass Defect-based Carbonyl Activated Tags (mdCAT) for Multiplex Data-independent Acquisition Proteome Quantification; Siwen Zhang1; Yi Di2; 1Shanghai Cancer Center and Institutes of Biomedical Sciences, Shanghai, China; 2Institute of Bioinformatics, ShanghaiTech University, Shanghai, China
MP 124  The influence of tissue content on proteomic variation in high-grade serous ovarian cancer; Srikanth S Manda; Maiken M Espersen; Rohan Shah; Steven G Williams; Natasha Lucas; Dylan Xavier; Sadia Mahboob; Andrew Robinson; Peter G Hains; Brett Tully; Roger R Redel; Philip J Robinson; Qing Zhong; Anna Defazio; Rosemary Balleine; 1Children’s Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; 2Centre 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; Timothy Man; Lucie Piecková; Lynn Verbeke; Maximilian J. Helf; Tejas Gandhi; Roland Bruderer; Lukas Reiter; Biognosys, Schlieren, Switzerland

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

MP 127  High dynamic range proteome analysis with BoxCar DIA and super-resolution Orbitrap mass spectrometry; Florian Meier; Kyle Fort; Arne Kreutzmann; Daniel Marc Mourtad; Konstantin Aizikov; Dmitry Grinfeld; Johannes B Mueller; André C Michaelis; Alexander A. Makarov; Matthias Mann; Max Planck Institute of Biochemistry, Planegg, Germany; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 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; Brett S Phinney; Maxence Le Vasseur; Michelle Salemi; Jodi Nunnari; UC Davis, Davis, CA

MP 129  Achieving true DIA analysis via 2DMS; Christopher Andrew Wootton; Tomas E. Morgan; Bryan P. Marzullo; Alina Theisen; Anisha Haris; Diana C. Palacio Lozano; Yuki Pui Yi Lam; Mark P. Barrow; Peter B O’Connor; University of Warwick, Coventry, United Kingdom

MP 130  KDM1A Inhibition Enhances ESR2-mediated Tumor Suppression in Ovarian Cancer; Prabhakar Pitta-Venkata; Yihong Chen; Bridgite Palacios; Ilanna Loeffel; Sammy Pardo; Dana Molleir; Ratna Vadlamudi; Susan T. Weintraub; Gangadhara Sareddy; 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; Roland Bruderer; Oliver M. Bernhardt; Lynn Verbeke; Sega Ndiaye; Claire Dauly; Lukas Reiter; Biognosys AG, Schlieren, Switzerland; 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; Gautam Saxena; Aleksandra Binek; Simion Kreimer; Aaron Robinson; Jennifer E Van Eyk; DeepDIA, Bethesda, MD; Cedars-Sinai Medical Center, Los Angeles, CA

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

MP 134  Data independent workflow using SWATH® acquisition for comprehensive cell culture media analysis; Zuzana Demianova; Elliott Jones; David Cox; Lei Xiong; Sciex, Brea, CA; SCIEX, Redwood Shores, CA; SCIEX, Concord, ON

MP 135  InfineQ: Real-time cloud-based DIA data processing for high-throughput proteomics; Artyom Pugachev; Arnaud Groen; ProteiQ Biosciences GmbH, Berlin, Germany

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

MP 137  Establishing the Clinical Relevance of Glycoproteins in Pancreatic Cancer; Tiffany Thein; Abel Bermudez; Jeremy Sharib; Sarah M Totten; Fernando Garcia-Marques; Tyler York; Keely Fuller; Kimberly S Kirkwood; Sharon J Pittel; Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; 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; Siu Kwan Sze; Nanyang Technological University, Singapore, Singapore

DISEASE BIOMARKERS

MP 137-162

MP 137  Damaged vascular ECM proteins induced cardiovascular diseases by recruiting macrophages and LDLs to atherosclerotic plaque; Siu Kwan Sze; Nanyang Technological University, Singapore, Singapore

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

ASMS 2020 Reboot  Page 13
Analysis of advanced glycation end products through LC-MS/MS for the early diagnosis of cancer: Lakmini Senavirathna1; Ru Chen2; Sheng Pan1; 1University of Texas Health Science Center at Houston, Houston, TX; 2Baylor College of Medicine, Houston, TX

Novel Spatial N-Glycomic and Glycocalyx Profile of 3D Human Colon Cancer Cell Lines Utilizing a NanoLC-MS Base Platform: Qing W Zhou1; Jennyfer Tena2; Carlito B Lebrilla3; 1University of California, Davis, Davis, CA

Metabolic rewiring Modulates amyloid-like aggregates formation in Huntington’s disease: Sai Manohar Thota1; Sai Sanwaid Pradhan2; Bhavana N Reddy2; Isha Verma3; Rajesh Babu D4; Vivek Tiwari5; Vidyasagar K6; Pavan Vasoya5; Ashish Pargaonkar2; Deepak Saligram2; Sunil H V6; Krishna Murty V3; Seshagiri Polan3; Sanjaya Viswamitra3; Dileep Kumar10; Joshy E V9; Venketheswara Sivaramakrishnan1; 1Department of Biosciences, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India; 2Department of Radiology, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India; 3Department of Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bengaluru, India; 4Department of Chemistry, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India; 5centre for Brain Research, Indian Institute of Science, Bengaluru, India; 6Department of Neurosurgery, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India; 7Agilent Technologies, BENGALURU, India; 8FDI + Care, Department of Nuclear Medicine and PET CT, Mazumdar Shaw Cancer Center, Bengaluru, India; 9Department of Neurology, Sri Sathya Sai Institute of Higher Medical Sciences, Bengaluru, India; 10Siemens Healthcare Pvt Limited, Bengaluru, India

Development of a high-content high-throughput screening platform using integrated omics to assess for impacts on metabolism: John Janiszewski1; Matt Hall1; Sam Michael2; Richard Schneider3; Stephen Ferguson2; Michael Iannotti1; Rebecca Cardone3; Richard G. Kibbey2; Raghav Sehgal2; Qiushi Sun3; Surbhi Poddar4; Maheswari Karthikeyan4; Sunil Dhakad5; Darren Dumlao6; Elias Padilha3; Kelli Wilson4; 1NIH/NCATS, Rockville, MD; 2NIH/NIEHS, Durham, NC; 3Yale University, New Haven, CT; 4Elucidata, Delhi, India; 5SCIEX, Redwood Shores, California 1201

Adenosine Deaminase reprograms metabolism and promotes onset and progression of Rheumatoid Arthritis (RA): Saikrishna Srimadh Bhagavathyam1; Dr. Narasimulu Gunda2; Dr. Narasimhan K3; Dr. Damodaram Potkuri4; Dr. Rajesh Babu Dandumudi5; Dr. Sai Mangala Divi6; Dr. Ashish Pargaonkar7; Dr. Rahul Ray8; Sujith Kumar Pulukool9; Dr. Vishnu Kannan10; Ashwin Ashok Naik1; Saibharathim Simha Reddy Santha1; Dr. Prakash Khanchandani1; Dr. Venketheswara Sivaramakrishnan1; 1Department of Biosciences, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India; 2GVN Medical Centre, Hyderabad, India; 3Sri Sathya Sai General Hospital, Puttaparthi, India; 4Subodhaya Rheumatology Centre, Tirupati, India; 5Department of Chemistry, Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India; 6Department of Biochemistry, Sri Sathya Sai Institute of Higher Medical Sciences, Puttaparthi, India; 7Agilent Technologies India Pvt Ltd, Bengaluru, India; 8Department of Orthopedics, Sri Sathya Sai Institute of Higher Medical Sciences, Prasantham Gram, Puttaparthi, India

Breath Biopsy: combining Thermal Desorption-Gas Chromatography with High Resolution Mass Spectrometry for improved sensitivity and selectivity in untargeted breath analysis: Dominic Roberts1; Lori Dolata2; Cristian Cojocariu3; Max Alisworth4; Jason Cole5; Paul Silcock6; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Redwood City, California 1201; 3Thermo Fisher Scientific, Austin, Texas; 4Owlstone Medical Ltd, Cambridge, United Kingdom; 5Thermo Fisher Scientific, Austin, Texas

Developing proteins and phosphoproteins in urine extracellular vesicles as biosignatures for Parkinson’s disease diagnostics: Marco Hadisurya1; Li Li2; Shalini Padmanabhan3; Anton Illiuik4; W. Andy Tao1; 1Purdue University, West Lafayette, IN; 2Tymora Analytical Operations, West Lafayette, IN; 3The Michael J. Fox Foundation, New York City, NY; 4Tymora Analytical, West Lafayette, IN

Robust Plasma Protein Profiling Workflow for Routine Clinical Research Using a UHPLC and a Modified Orbitrap Mass Spectrometer: David Sarracino1; Christian Klaas2; Bradley J Hart2; Shen Luan1; Amol Prakash3; Xiaolei Xie4; Debadeep Bhattacharyaa4; 1Thermo Fisher Scientific, Cambridge, MA; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3ThermoFisher Scientific, San Jose, CA; 4Optyx Tech Corporation, Shrewsbury, MA; 5Thermo Fisher Scientific, San Jose, California

Mass spectrometry-based proteomics of liquid biopsies for neurodegenerative diseases screening: Svitlana Rozanova1; Katarin Barkovits2; Katrin Marcus1; 1Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany

Top-down LC/MS Analysis of Cardiac Troponin I Proteoforms from Clinical Blood Samples of Acute Myocardial Infarction: Timothy Tiambeng1; David S Roberts1; William H. Swain2; Daniel Kim3; Song Jin4; Ying Ge1; 1Chemistry Department University of Wisconsin-Madison, Madison, WI 53705; 2University of Wisconsin School of Medicine and Public Health, Madison, WI; 3Human Proteomics Program, School of Medicine and Public Health, Madison, WI; 4Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI

Identification of Biomarkers for Glioblastoma in Saliva using UPLC-IM-MS: Amy N. W. Schnelle1; Christina A. Gaw1; Luke T. Richardson2; Fengfei Wang2; Exri Wu2; Touradj Solouki1; 1Baylor University, Waco, TX; 2Neuroscience Institute and Department of Neurosurgery, Baylor Scott & White Health, Temple, TX
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**MP 151** Proteomic Profiling of Extracellular Vesicles Isolated from Human Alzheimer’s Disease Brain Tissues; Manveen K Sethi1; Satoshi Muraoaka1; Annina M. Deleo1; John D. Hogan1; Tsuneya Ikeyu1; Joseph Zaia1; 1Boston University School of Medicine, Boston, MA

**MP 152** Protein Signatures to Distinguish Aggressive from Indolent Prostate Cancer; Fernando Garcia-Marques1; Shiqin Liu1; Sarah M Totten1; Abel Bermudez1; Rosalie Nollely; Cheylene Tanimoto1; En-Chi Hsu1; Tanya Stoyanova1; James D. Brooks1; 2; Sharon J Pfitzen1; 1Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; 2Department 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; Kelly Servage1; Karolina Stefan01; Kim Orth1; 1UT 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 Borkar1; Shiva Shankar Ravi1; Danthasinghe Waduge Badrajeey Piyanatthan1; Karthik Reddy Kam Reddy1; Dimuthu Perera1; Martha K Terr1; Kimiko L Krieger1; Roni J Bollag2; Stephen B Williams3; Kimal Rajapaksha4; Leomar Y Ballester4; Balasubramanyam Karanam5; Shym M. Kavuri1; MinjiaLee6; Arun Sreekumaran7; Yair Lotan8; Cristian Coarfa9; Nagireddy Putluri1; 1Baylor College of Medicine, Houston, TX; 2Augusta University, Augusta, GA; 3University of Texas Medical Branch at Galveston, Galveston, TX; 4University of Texas at Houston Health Science Center, Houston, Texas; 5Tuskegee University, Tuskegee, AL; 6University of Texas Health Science Center at Houston, Houston, TX; 7UT Southwestern Medical Center, Dallas, TX

**MP 157** Proteomics Studies in Parkinson’s Disease; George S. Katselis1; Paulos Chumala1; Brooke Thompson1; Savannah Eanes1; Sarah Bocking1; Alex Rajput1; Ali Rajput1; 1University of Saskatchewan, Saskatoon, SK

**MP 158** Redox regulation of glutathione per/polysulfide in hyperglycemic endothelial cells; Xinggui Shen1; Christopher G. Kevil1; 1Department 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 Iles1; Ray Iles2; George Carney1; Raminta Zmuina1; Alexander Sampson1; Matteo Ferrari1; Angalee Nadesalingam1; Sneha Vishwanath1; Jonathan Heeney1; 1University of Cambridge, Cambridge, United Kingdom; 2MAP Sciences, Bedford, United Kingdom; 3DIOSynVax, 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; Roman V. Koziy1; Paulos Chumala2; Elemir Simko1; Georgios S. Katselis2; 1Department of Pathology, Western College of Veterinary Medicine, University of Saskatchewan, Saskatoon, SK; 2Department 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; Clizia Chinello1; Noortje De Haan2; Giulia Capitoli3; Barbara Trezzi4; Antonella Radice5; Stefania Galimberti3; Manfred Wuhrer2; Renato Alberto Sinico5; Fulvio Magni6; 1Clinical Proteomics & Metabolomics Unit, Dep. of Medicine and Surgery, UNIMIB, Vedano al Lambro, Italy; 2Department of Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; 3Centre of Biostatistics for Clinical Epidemiology, Dep. of Medicine and Surgery, UNIMIB, Monza, Italy; 4Nephrology Unit, Dep. of Medicine and Surgery, UNIMIB, Monza, Italy; 5Microbiology and Virology Department, San Carlo Borromeo Hospital, Milan, Italy; 6Clinical Proteomics & Metabolomics Unit, UNIMIB, Dep. of Medicine and Surgery, Vedano al Lambro, Italy

**DRUG DISCOVERY/DMPK/ADME I**

**MP 163-174**

**MP 163** A novel G protein-biased and subtype selective agonist for a G protein-coupled receptor discovered from screening herbal extracts; Bingjie Zhang1; Simeng Zhao1; Ye Xin1; Wening Shui1; 1Human 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; Nicole Bebrin1; Linlin Dong1; Kojo Abdul-Hadi1; Robert Griffin1; Dong Wei1; Mark G Qian1; 1Takeda 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; Jean Lacoursière1; Serge Auger1; Francis Bréere2; Pier-Luc Plante2; Pierre Picard1; 1Phytronix Technologies, Québec, QC; 2Université Laval, Québec, Québec

**MP 166** Ultra High-Throughput and Chromatography-Free Bioanalysis of Polar Analytes with Acoustic Ejection Mass Spectrometry; Andrew Wagner1; Jun Zhang1; Chang Liu2; Tom Covey2; Timothy Olah1; Harold Weller1; Wilson Shou1; 1Bristol-Myers Squibb, Princeton, NJ; 2SCIEX, Concord, ON

**MP 167** Assaying Protein / Ligand Binding with High-Resolution Native Mass Spectrometry; Matthias Witt1; Christopher Thompson1; Yongwei (peter) Wang2; Michael Greig3; Marshall W. Bern4; Xuefei Yin5; Ilker Sen6; Jia Liu6; Yang Ye6; 1Bruker Daltonic GmbH, Bremen, Germany; 2Bruker Scientific LLC, Billerica, MA; 3Bruker
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Daltonics, shanghai, China; *Bruker Scientific, San Jose, CA; 2Protein Metrics, Cupertino, CA; 3Shanghai 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 Ji1; Xueyuan Zhang1; Jinzhi Liu1; Yu Chen1; Ji Liu1; Chunlei Li1; Min Meng1; Laixin Wang1; 1Chongqing Denali Medpharma Co., Ltd, Chongqing, China; 2CSPC Pharmaceutical Group Ltd, Shijiazhuang, China

MP 169 Measurement of Free Concentrations of Testosterone Using Newly Developed SpinTip Microextraction Devices with Polycrylonitrile: Daniel Galke1; F. Marcel Musteata1; 1Albany College of Pharmacy and Health Sciences, Albany, NY

MP 170 LC-MS/MS quantitation of Wthaferin A and 12-Deoxywthaframolde in mouse plasma and brain following oral administration of ashwagandha herbal extract solution: Ludmila Alexandrova1; Zhiyong Xie1; Edwin Chang2; Chirag B. Patel2; 3Corinne Beinan2; Luis Avila2; Lal Hingoran2; Sanjiv S. Gambhir2; 6Allis S. Chien1; 1Stanford University Mass Spectrometry, Stanford University, Stanford, CA; 2Department of Radiology, Molecular Imaging Program at Stanford (MIPS), Stanford University School of Medicine, Stanford, CA; 3Department of Neurology and Neurological Sciences, Stanford University School of Medicine, Stanford, CA; 4Avetia Biomics, Bedford, MA; 5Pharmenza Herbal Pvt Ltd, Kansari, India; 6Department of Bioengineering, Stanford University, Stanford, CA; 7Department 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: Hong Tsao1; Scott Carrier1; Joseph Janiszewski2; Wayne Lootsma2; Steve Ainsley2; 1Vertex Pharmaceuticals, Boston, MA; 2Sound Analytics, Niantic, CT

MP 172 Proteolytic activity of enzyme beta lytic metalloendopeptidase as a potential antibacterial agent: Mihail Konstantinov1; 2Alexey Afoshin3; Irina Kudryakova4; Natalia Vasilyeva4; Ilya Toropygin4; 1Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; 2Pirogov Russian National Research Medical University, Moscow, Russia; 3G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Pushchino, Russia; 4Orekhovich Institute of Biomedical Chemistry, Moscow, Russian Federation

MP 173 QTAP analysis of transporters for validation of human brain microvascular endothelial cell line as an in vitro human BBB model: Mouhssin Oufir1; Jordan Goncales1; Gregory Harichaux1; Yann Courbebaisse1; Isabelle Seibert1; Henriette Meyer Zu Schwabedissen2; Fabrice Viviani3; Matthias Hamburger3; Oncodesign, Villebon-Sur-Yvette, France; 2ADOCIA, LYON, France; 3UNIVERSITY OF BASEL, BASEL, Switzerland

MP 174 The novel data-mining strategy for metabolite identification based on UHPLC-Q-Exact hybrid quadrupole orbitrapHRMS: Application to Prucalopride: Lihua Zuo1; Liwei Liu2; Yingying Shi2; Zhuolun Li2; Xiaojian Zhang2; Zhi Sun2; 1The First Affiliated Hospital of Zhengzhou University, Zhengzhou, China; 2The First Affiliated Hospital of Zhengzhou University, Zhengzhou, China

ELEMENTAL ANALYSIS: ICP/MS

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

MP 176 Using ICP-MS/MS with M-Lens for the analysis of high silicon matrix samples: Yu Ying1; Xiangcheng Zeng1; 1Agilent 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): Ashley Parisi-Goldblatt1; James Henderson1; Evan Ray1; Howard M. Kingston3; 1Duquesne University, Pittsburgh, PA; 2University of Pittsburgh, Pittsburgh, PA

MP 178 An Innovative Platform Merging Elemental (LA-ICP-MS) and Biochemical (FTIR Imaging) Analysis for Biological Tissues; Khalid A. Al-Saady1; Fadl Rakti1; Mohamed Ali2; Rafif Al-Saady3; Erik Goormaghtigh4; 1Qatar University, Doha, Qatar; 2Qatar Biomedical Research Institute, Doha, Qatar; 3Al Ahi Hospital, Doha, Qatar; 4Université Libre de Bruxelles, Brussels, Belgium

MP 179 Simultaneous Determination of Heavy Metal and Mineral Content in Fruit Juices by Inductively Coupled Plasma Mass Spectrometry: Raymond Li1; Regina Tan2; Zhaoqi Zhan1; 1 Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; 2National University of Singapore, Singapore
Cryofocus fast gas chromatography combustion isotope ratio mass spectrometry featuring a low temperature catalytic combustion reactor; Ri Scott Lacombe\textsuperscript{1}; Andrew Jones\textsuperscript{2}; J. Thomas Brenna\textsuperscript{1}; Herbert J Tobias\textsuperscript{1}; \textsuperscript{1} Dell Pediatric Research Institute, University of Texas at Austin, Austin, TX; \textsuperscript{2} Activated Research Company, Eden Prairie, MN

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\textsuperscript{1}; Konstantin O. Nagornov\textsuperscript{2}; Anton N. Kozhinov\textsuperscript{2}; Yury O. Tsybin\textsuperscript{2}; Tyler J. Williams\textsuperscript{1}; R. Kenneth Marcus\textsuperscript{1}; \textsuperscript{1} Clemson University, Clemson, SC; \textsuperscript{2} Spectroswiss, Lausanne, Switzerland

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

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

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

Time-resolved time-of-flight secondary ion mass spectrometry for in-situ characterization of functional materials; Anton Ievlev\textsuperscript{1}; Olga S. Ovchinnikova\textsuperscript{2}; \textsuperscript{2} Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; \textsuperscript{3} Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

Resonance Ionization Mass Spectrometry for trace analysis of solids: depth profiling with flat-top laser ablation probe; Igor V. Veryovkin\textsuperscript{1}; Olga S. Ovchinnikova\textsuperscript{2}; \textsuperscript{1} University of Illinois at Chicago (UIC), Chicago, IL; \textsuperscript{2} Arizona State University, Tempe, AZ 85287; \textsuperscript{3} California Institute of Technology, Pasadena, CA

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

Towards development of a matrix-independent calibration strategy for targeted quantification of milk allergens; Bini Ramachandran\textsuperscript{1}; Charles Yang\textsuperscript{2}; Melanie Downs\textsuperscript{1}; \textsuperscript{1} University of Nebraska-Lincoln, Lincoln, NE; \textsuperscript{2} Thermo Fisher Scientific, San Jose, California

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

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

Quantitative Analysis of Blended Oils by Matrix-assisted Laser Desorption/Ionization Mass Spectrometry and Partial Least Squares Regression; Suying Li\textsuperscript{1}; Tsz-Tsun Ng\textsuperscript{1}; Zhong-Ping Yao\textsuperscript{1}; \textsuperscript{1} The Hong Kong Polytechnic University, Hong Kong, Hong Kong

Metabolomics profiling for identification of the bioactive constituents in Taiwan aboriginal herb using high-resolution mass spectrometry; Hong-jhang Chen\textsuperscript{1}; GUI-RU Xie\textsuperscript{1}; \textsuperscript{1} National Taiwan University, Taipei, Taiwan

Evaluating the quantification of soy protein in incurred matrices using a targeted LC-MS/MS method; Jenna Krager\textsuperscript{1}; Joseph L. Baumert\textsuperscript{1}; Melanie L. Downs\textsuperscript{1}; \textsuperscript{1} University of Nebraska-Lincoln, Lincoln, NE
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MP 194  Targeted Peptide Quantitation of Seven Food Allergens in Dark Chocolate Using Triple Quadrupole LC/MS; Lee Sun Ney1; Jerry Zweigenbaum2; Chee Sian Gan1; 1Agilent Technologies Singapore (Sales) Pte Ltd, Singapore, Singapore; 2Agilent Technologies, Wilmington, DE

MP 195  Quantitation of Patulin in Apple Juice and Apple Products using a compact mass spectrometer; Daniel Eikel1; Changtong Hao1; Simon Prosser1; 1Advion Inc., Ithaca, NY

MP 196  Peanut Allergens Survive Excessive Dry Thermal Processing; Lee K Palmer1; Justin T Marsh1; Joseph L Baument1; Philip E Johnson1; 1University of Nebraska-Lincoln, Lincoln, NE

MP 197  Structure elucidation of ultra-trace monoenes in milk and polyunsaturated PUFA with fragmentation rules by solvent-mediated covalent adduct chemical ionization MS/MS; Donghao Wang1; Zhen Wang1; J. Thomas Brenn11; 1University of Texas at Austin, Austin, Texas

MP 198  Developing an open real-time spectroscopic strategy for better understanding of food metabolomics; Ruey Leng Loo1,2; Samantha Lodge3,4; Berin Boughton5; Melvin C.L. Gay4; Heino M. Heyman6; Christopher Thompson7; Elaine Holmes1,8; Jeremy Nicholson1,9, 1Australian National Phenome Centre, Murdoch University, Murdoch, Australia; 2Research and Innovation Office, Murdoch University, Murdoch, Australia; 3Health Futures Institute, Murdoch University, Murdoch, Australia; 4Bruker Pty Ltd, Victoria, Australia; 5Bruker Daltonics, Billerica, MA

MP 199  Development of a real-time direct-MS screening technique for common adulteration and contamination scenarios in edible oils; Sara Stead1; Nicola Dreolin1; Pierre-Alain Golay2; Francesca Giuffrida2; Kornel Nagy3; Lindsay Hatch4; Kenneth Rosnack5; 1Waters Corporation, Wilmslow, United Kingdom; 2Societe des Produits Nestle S.A., Lausanne, Switzerland; 3Waters Corporation, Beverly, MA; 4Waters Corporation, Milford, MA

MP 200  Classification of Bacterial Strains with the Multi-ionization Platform and Open Mass Fingerprinting Framework (OMFF); Abigail Moreo-Pedraza1,2; Darrell D. Marshall3,4,5; Sandra Martinez-Jarquin3; Santosh Kar1,6; Khoa Hoang7; Milan Popovic3; Vladimir Shulaev2; Charles N. McEwen8; Robert Winkler1; Sarah Trimpin1,9; 1University of Nebraska-Lincoln, Lincoln, NE; 2University of Texas at Austin, Austin, Texas; 3Agilent Technologies, Redwood City, CA; 4Total Analysis LLC, Newark, Delaware; 5Bruker Pty Ltd, Victoria, Australia; 6Australian National Phenome Centre, Murdoch University, Murdoch, Australia; 7Bruker Daltonics, Billerica, MA; 8University of North Texas, Denton, TX; 9Department 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 Nieto1; Melissa Cheruy2; 1Agilent Technologies, Inc., Santa Clara, CA

MP 202  Post-harvest influences volatile aroma profiles of melon varieties identified by HS-SPME-GC-MS; Varsha Ravi1; Jasbir Singh2; Rita Metrani2; G. K. Jayaprakash2; Bhimanagouda S. Patil2; 1Texas A&M university, College station, TX; 2Texas A&M University, College Station, TX

MP 203  Widely targeted metabolomics of hydrophilic compounds using LC-MS/MS-HRMS-MS -How compounds change when curry is stored overnight?; Takanari Hatton1; Harumi Kubo1; Yasuko Yamada1; Jun Watanabe1; 1Shimadzu Corporation, Kyoto, Japan; 2Shimadzu Techno-Research, Inc., Kyoto, Japan

MP 204  Nontargeted and Statistical Approaches for Honey Authenticity Analysis; Katherine Hyland1; Diana Tran2; 1Shimadzu Corporation, Hadano, Japan; 2Shimadzu Corporation, Kyoto, Japan

MP 205  Highly sensitive analysis of the related substance of ciguatoxins by the multiple reaction monitoring and electrospray ionization with LC/MS/MS; Manami Kobayashi1; Kota Ishioka1; Junichi Masuda1; Yoshihiro Hayakawa2; 1Shimadzu Corporation, Hadano, Japan; 2Shimadzu 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 Xiong1; Christine H. Parker1; Catherine L. Fiedler1; 1U.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 Guo1; Lijun Li1; Nick Zhu2; Rui Gong2; Zong Yang1; 1Shimadzu Corporation, Yokohama, Japan; 2Wuhan Institute for Food and Cosmetic Control, Wuhan, China

FUNDAMENTALS: PHOTODISSOCIATION

MP 208  Wavelength-Tunable Ultraviolet Photodissociation for Structural Analysis of Unsaturated Lipids; Hai-Fang Li1; Jing Zhao1; Wenbo Cao1; Yu Xia1; Zheng Ouyang1; 1Department of Precision Instrument, Tsinghua University, Beijing, China; 2Department of Chemistry, Tsinghua University, Beijing, China

MP 209  Differentiation of Peptide Isomers by Modulated Excited-State Dissociation; Brielle L. Van Orman1; Hoi-Ting Wu1; Ryan R. Julian1; 1University of California, Riverside, Riverside, CA

MP 210  Probing Proline Cis/Trans Isomer Scrambling During ESI With Radical-Directed Dissociation; Jacob W Silzle1; Miklos Guttman2; Ryan R. Julian3; 1UC Riverside, Riverside, CA; 2University of Washington, Seattle, WA; 3University of California, Riverside, Riverside, CA
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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 Grottemeyer; Christian-Albrechts-Univ, Kiel, Germany

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

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

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

GLYCOPROTEINS I

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

MP 216 A workflow for the Large Scale Quantitative Proteomics and N-Glycoproteomics Analysis of Cancer Cells; Xiaoju Tian; Ping Wu; Chen Su; Yue Yin; Chao Peng; 1National 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; Zhengwei Chen; Xiaofang Zhong; Lingjun Li; 1University of Wisconsin-Madison, Madison, WI

MP 219 Simple and fast assay for apolipoprotein E phenotyping and glycootyping: Discovering isoform-specific glycosylation in plasma and cerebrospinal fluid (CSF); Yueming Hu; Hussein N Yassine; Dobrin Nedelkov; 1Isoformix Inc., Phoenix; 2University 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; Jonathan Jones; Peter Haberl; Maurizio Bronzetti; 1Genedata AG, Basel, Switzerland; 2Genedata Ltd, Cambridge, United Kingdom; 3Genedata GmbH, Munich, Germany; 4Genedata 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; Ming Tong; Suttipong Suttapitugsakul; Ronghu Wu; 1Georgia Institute of Technology, Atlanta, GA

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

MP 223 Comprehensive Analysis of IgE Glycoforms by FAIMS-LC-MS/MS using Orbitrap Eclipse Mass Spectrometer; Aman Makaju; Kim Alving; Bing Wang; Rosa Viner; 1ThermoFisher Scientific, San Jose, CA; 2Sanoft, 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; Lei Tao; William Alley; 1Chunming Yao; 2Ying Qing Yu; Weibin Chen; 1Waters Corporation, Milford, Massachusetts; 2National Institute for Food and Drug Control, Beijing, China; 3Texas A&M University - San Antonio, San Antonio, TX

MP 225 N-Linked Glycoproteome Analysis of Bovine Milk Exosomes; Xuyao Zeng; Brooke A. Brown; Kathleen T. Grassmyer; Jonathan C. Trinidad; 1University of California Davis, Davis

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; Somak Ray; Shuiliu Lu; Jennifer Jones; Ionita Ghiran; 1Barnett Inst., Northeastern University, Boston, MA; 2Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA; 3NIH/NCI/CCR, Bethesda, MD

MP 227 Glycomic and Glycoproteomic Analysis of Brain N-Glycosylation in High Fat Diet-Induced Obese Mice; Mackenzie Honeycutt; Jennyfer Tenas; Amanda Krueger; Helen Raybould; 1University 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; Erika Cline; Shengkun Dai; Steven Patrie; 1Northwestern University, Evanston, IL
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MP 229 Metabolic Engineering Challenges to extending N-glycan pathways in CHO cells; Qiong Wang1; Tiexin Wang2; Shuang Yang3; John Cipollo4; Michael J. Betenbaugh5; 1JHU Chemical Engineering Department, Baltimore; 2JHU Chemical Engineering Department, Baltimore, Maryland; 3FDA Laboratory for Bacterial Polysaccharides, Silver Spring, Maryland

MP 230 Depleting Depletion and Fractionation for Deep Site-Specific Profiling of the Urinary Glycoproteome; John Froehlich1; Shannon E. DiMartino2; 1Boston Childrens Hospital, Boston, MA; 2Boston 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 Sanda1; Julius Benicky1; Zuzana Brnakova Kennedy1; Radoslav Goldman1; 1Georgetown 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 Eckmair1; Chunsheng Jin2; Daniel Abed-Navandi3; Iain B. H. Wilson1; Katharina Paschinger1; 1University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria; 2Goteborgs universitet, Goteborg, Sweden; 3Haus des Meeres - Aqua Terra Zoo, Vienna, Austria

MP 234 New insights into the honeybee N-glycome by off-line LC-MS analysis; Alba Hykollari1; Daniel Malzl2; Jorick Vanbeselaere2; Barbara Eckmair2; Iain B. H. Wilson2; Katharina Paschinger2; 1Vetcore, Proteomics Facility, Veterinärmedizinische Universität Wien, Wien, Austria; 2Department 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. Drinkard1; Kaitlin Hoyt1; Susanne R. Kalb1; John R Barr1; 1Centers For Disease Control and Prevention, Atlanta, GA

MP 236 Improving the detection of molecular indicators of Abrus precatorius with LC-MS; Christina S Robb1; Kirk W Gaston2; Alexis G Mazurek3; 1The Connecticut Agricultural Experiment Station, New Haven, CT; 2FDA Forensic Chemistry Center, Cincinnati, Ohio; 3University of New Haven, New Haven, CT

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MP 237-244

MP 237 Matrix sublimation device with recrystallization system for MALDI mass spectrometry imaging; Vasily Eliferov1; Andrey Shivalin1; Daniil Ivanov1; Eugene Nikolaev2; Igor Popov1; 1Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 2Skolkovo 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 Mueller1; Dhaka Ram Bhandari1; Kerstin Strupat1; Bernhard Spengler1; 1Justus Liebig University, Giessen, Germany; 2Thermo 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 Saigusa1; Ritsumi Saito1; Komei Kawamoto2; Akira Uruno1; Kuniyuki Kano2; Junken Aoki1; Masayuki Yamamoto1; Tadafumi Kawamoto2; 1Tohoku University, Sendai, Japan; 2Tsurumi 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 Colley1; Sitai Liang2; Chunyan Tan2; Kyle P. Troubough2; Stephen B.H. Bach3; Yong-Hee Patricia Chun2; 1University of Texas, Texas, San Antonio, TX; 2UT Health San Antonio, Department of Periodontics, San Antonio, TX; 3University of Texas in San Antonio, San Antonio, TX; 4UT 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 Patel1; Kevin Randall1; Cathy Merry2; Philippa J Hart3; 1Medicines Discovery Catapult, Alderley Edge, United Kingdom; 2University of Nottingham, Nottingham, United Kingdom

MP 243 Systematic Evaluation of Analyte Delocalization in Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging; Eric S Barton1; Caitlin M. Tressler2; Kristine Glunde2; 1Johns Hopkins University School of Medicine, Baltimore, MD; 2Johns 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 Fourmelle1; Ethan Yang2; Martin Dufresne3; Pierre Chaurand1; 1Department of Chemistry, University of Montreal, Montréal, QC; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205
INFORMATICS: METABOLOMICS
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MP 256  High-Throughput Metabolite Profiling for Synthetic Biology using Ion Mobility-Mass Spectrometry and Data-Independent Acquisition with Improved Targeted Data Extraction Software; Aivelit Bilbao1; Nathalie Munoz1; Daniel J. Orton1; Xueyin Zheng1; Karl K. Weitz1; Kyle Pomraning1; Shuang Deng1; Beth Hofstad1; Ziyu Dai1; Alex Apffel2; Richard D. Smith1; Young-Mo Kim1; Jon Magnuson2; Kristin E. Burnum-Johnson1; 1Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington; 2Chemical and Biological Processes Development Group, Richland, Washington; 3Agilent Technologies, Santa Clara, CA

MP 257  Exploring DIA data analysis for metabolomics with Spectronaut; Maximilain J. Helf1; Kathleen Rousseau2; Oliver M. Bernhardt1; Tejas Gandhi1; François Fenaillée2; Lukas Reiter1; 1Biognosys, Schlieren, Switzerland; 2Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France

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Fingerprint-decoding neural networks enable database-independent compound generation from fragment spectra; Michael Andrej Strav1, 2; Kai Dührkop1; Heinz Singer1; Sebastian Böcker2; Nicola Zamboni1; 1ETH Zurich, Zurich, Switzerland; 2ETH Zurich, Zurich, Switzerland

Comparing accurate mass MS/MS spectral similarity algorithms for small molecules; Yuanyue Li1; Tobias Kind1; Oliver Fiehn1; 1NIH West Coast Metabolomics Center, UC Davis, Davis, California

Mass spectrometry searches using MASST; Mingxin Wang1, 2; Alan K. Jarmusch1; Fernando Vargas1; Alexander A. Aksenov1; Julia M. Gauglitz1; Kelly Weldon1; Daniel Petras1; Ricardo Silva1; Robert Quinn1; Alexey Melnik1; Justin Van Der Hooft1; Andres Caraballo-Rodriguez1; Louis-Felix Nothias1; Christine Aceves1; Morgan Panitchpadhi1; Elizabeth Brown1; Francesca Di Ottavio1; Nicole Sikora1; Emmanuel Elijah1; Lara Labarta-Bajo1; Emily Gentry1; Shabnam Shalapour1; Kathleen Kyle1; Sara Puckett1; Jeramie Watrous1; Carolina Carpenter1; Amina Bouslimani1; Madeleine Ernst1; Austin Swafford1; Elna Zuniga1; Marcy Balunas6; Johnathan Klassen6; Rohit Loomba1; Rob Knight1; Nuno Bandeira1; Pieter C. Dorrestein1; 1UCSD, La Jolla, CA; 2Ometa Labs, San Diego, CA; 3Collaborative Mass Spectrometry Innovation Center, University of California San Diego, La Jolla, CA; 4Michigan State University, East Lansing, MI; 5Wageningen University and Research, Wageningen, Netherlands; 6University of Connecticut, Storrs, CT

Crossing the Chasm: One integrated solution for advancing LC-PASEF based pharma, metabolomics, non-target screening and exposome research; Xuejun Peng1; Guillaume Tremintin1; Heiko Neuweger2; Aiko Barsch2; Heino M. Heyman3; Sofie Weinkouff3; Nikolas Kessler2; 1Bruker Daltonics, San Jose, CA; 2Bruker Daltonik GmbH, Bremen, Germany; 3Bruker Daltonics, Billerica, MA

Combining Chromatographic Deconvolution with Electron Ionization and Chemical Ionization for Unknown Identification with High-Resolution Accurate Mass GC/MS; Dominic Roberts1; Jason Cole2; Xin Zheng2; John Voss3; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Austin, TX

molDiscovery: learning mass spectrometry fragmentation; Liu Cao1; Alexey Gurevich2; Hosein Mohimani1; 1Carnegie Mellon University, Pittsburgh, PA; 2St. Petersburg State University, St. Petersburg, Russia

MetaboDashboard: A simple machine learning pipeline and visualisation tool for metabolomics applied to diet profiles; Francis Briere1; Nancy Bouche2; Pier-Luc Plante1; Jacques Corbeil1, 2; Didier Brassard2; Benoit Lamarche3; 1Université Laval, Québec, QC; 2CHU de Québec-Université Laval, Quebec, Qc; 3Institute of Nutrition and Functional Foods, Quebec, Qc

Automated Metabologenomics Pipeline for Scalable Non-Ribosomal Peptide (NRP) Discovery Finds NRPs Produced by Soil and Human Skin Microbes; Bahar Behsaz1; Alexey Gurevich2; Amina Bouslimani3; Rob Knight4; Pieter C. Dorrestein1; Hosein Mohimani1; Pavel A. Pevzner1; 1UC San Diego, La Jolla, CA; 2St. Petersburg State University, St. Petersburg, Russia; 3University of California San Diego, San Diego, CA; 4Carnegie Mellon University, Pittsburgh, PA

An underappreciated challenge in identifying metabolites: scoring matches between library spectra and LC-MS HRAM metabolite spectra from complex samples; Lewis Y. Geer1; Yamil Simón-Manso1; Xiaoyu Yang1; Stephen E. Stein1; 1NIST, Gaithersburg, MD

mzRAPP – enabling routine performance checks of non-targeted data pre-processing in LC-HRMS; Yasin El Abiead1, 2, 3; Maximillian Milford1; Gunda Koellensperger1, 2, 3; 1University of Vienna, Department of Analytical Chemistry, Vienna, Austria; 2Chemistry meets Microbiology, University of Vienna, Vienna, Austria; 3Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria

In-source CID ramping (InCIDR) and Co-variant ion analysis of hydrophilic interaction chromatography (HILIC) metabolomics; Eric Chiles1; Sara Maimouni1; Fredric E. Wondisford1; Wei-Xing Zong1; Chi Song2; Xiaoyang Su1; 1Rutgers University, New Brunswick, NJ; 2The Ohio State University, Columbus, OH

PAVE: an isotope labeling-based peak annotation engine for microbial metabolomics data analysis; Wenyun Lu1; Lin Wang1; Xi Xing1; Li Chen1; Joshua D. Rabinowitz1; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Austin, TX

SIRIUS 4: A fully automated workflow from feature detection to compound identification; Martin A Hoffmann1; Kai Dührkop2; Marcus Ludwig2; Markus Fleischauer2; Sebastian Böcker2; 1Friedrich-Schiller-University Jena, Jena, Germany; 2Friedrich-Schiller University of Jena, Jena, Germany

Considerations in the chromatographic processing of >100,000 retention indexed plant metabolomics GC-MS files by Genedata Expressionist; Brian M. Ruddy1; Joseph D. Shambaugh2; David A. Curiel1; Teresa K. Harp3; Jan P. Hazenbroek1; 1Corteva Agriscience, Johnston, IA; 2Genedata, Lexington, MA

Polly-PeakML: Uncovering the dark-matter of metabolomic space using a novel machine-learning algorithm for peak classification; Richa Mudit1; Kailash Yadav1; Saiful Bari Khan1; Shashank Jatav1; Kelly Marsh1; Brian Dranka2; Abhishek Jha3; 1Elucida, Delhi, India; 2Agios Pharmaceuticals, Inc., Cambridge, MA; 3Elucida, Cambridge, MA
SIFTER: Chemical Class Prediction of Unknown Biomolecules Using Ion Mobility-Mass Spectrometry and Machine Learning; Jaqueline A. Picache1; Jody C. May1; John A. McLean1; 1Vanderbilt University, Nashville, TN
### INSTRUMENTATION: GENERAL

#### MP 276
**Biological Detection by Trapped Particle Fluorescence**

Nathan a Grimes¹; Theresa Nguyen²; ¹University of South Florida, Tampa, FL; ²University of South Florida, Tampa

#### MP 277
**Quantification of microparticles through a quadrupole-ion-trap mass spectrometer**

Chun-Jen Hsiao¹; Jung-Lee Lin¹; Abdil Özdemir²; Chung-Hsuan Chen¹; ¹Academia Sinica, Taipei, Taiwan; ²Sakarya university, Adapazan, 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. Sanders¹; Virginia K. James¹; Konstantin Ayzikov²; Kyle L. Fort²; Dmitry Grinfeld²; Alexander Makarov²; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Thermo Fisher Scientific, Bremen, Germany

#### MP 279
**Resonance-Enhanced Detection of Metals in Aerosols using Single Particle Mass Spectrometry**

Sven Ehrlert¹; ²; Johannes Passig³; ⁴; Julian Schade³; ⁴; Ellen Iva Rosewig³; ⁴; Robert Irisig¹; ²; Thomas Kröger-Badge²; ⁴; Hendryk Czech²; ⁴; Martin Skoriz³; Thorsten Streibel³; ⁴; Lei Li³; Zhen Zhou³; Xue Li³; Henrik Fallgren²; Jana Moldanova³; Stefan Zimmermann³; ⁴; ¹Photolon GmbH, Schwerin, Germany; ²Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University Rostock, Rostock, Germany; ³Joint Mass Spectrometry Centre, Cooperation Group Comprehensive Molecular Analytics (CMA), Helmholtz Zentrum München, Neuperberg, Germany; ⁴Department Life, Light & Matter, University of Rostock, Rostock, Germany; ²Hexin Instrument Co., LTD, Guangzhou, China; ³IVL Swedish Environmental Research Institute, Gothenburg, Sweden

#### MP 280
**Numerical and experimental investigation of an rf-ion funnel**

Laurent Bernard¹; Loukas Kyriakidis¹; Philipp Krah¹; Paul Fremdling²; Stephan Rauschenbach²; Julius Reisse²; ¹Technical University Berlin, Berlin, Germany; ²University of Oxford, Oxford, United Kingdom

#### MP 281
**Highly flexible experiment design using XML control of a Q-cyclic IMS-ToF**

Jason L. Wildgoose¹; James I Langridge¹; Darren Hewitt¹; Paul Doorbar¹; David Harker¹; Konstantinos Thalassinos²; ³Waters Corporation, Wilmslow, United Kingdom; ¹University College London, London, United Kingdom; ²University of Oxford, Oxford, United Kingdom; ³Birkbeck 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 Bergen¹; Michael Goodwin¹; Helene Cardasis¹; Jesse D Canterbury¹; Graeme Mcalister¹; Michael W. Senko¹; Shannon Eluk¹; Vlad Zabrouska³; Romain Huguet¹; ¹Thermo 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 Ueda¹; Takanari Hattori¹; Wataru Fukui¹; Tsubasa Ibushi³; Kazuo Mukaibatake¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Techno-Research, Inc., Kyoto, Japan

#### MP 285
**Determination of contaminants when calibrating an Orbitrap Mass Spectrometer And How to Avoid Them**

Erik P.A. Couzijn¹; Siegrun A.I. Mohring¹; Ioanna Ntai²; ¹Photonion GmbH, Schwerin, Germany; ²Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University Rostock, Rostock, Germany; ³Joint Mass Spectrometry Centre, Cooperation Group Comprehensive Molecular Analytics (CMA), Helmholtz Zentrum München, Neuperberg, Germany; ⁴Department Life, Light & Matter, University of Rostock, Rostock, Germany; ²Hexin Instrument Co., LTD, Guangzhou, China; ³IVL Swedish Environmental Research Institute, Gothenburg, Sweden

#### MP 286
**A tandem instrument for measuring ion mobility separation and cross-section collision determination**

Jakub Ulma¹; Kevin Giles¹; Jason L. Wildgoose¹; David Langridge¹; Keith Richardson¹; Alistair Schofield¹; Witold Niklewski¹; ¹Waters Corporation, Wilmslow, United Kingdom

#### MP 287
**A Proteomic Sample Preparation for Mass Spectrometry Using an Automated Workstation**

Qin Fu¹; Casey W Johnson¹; Bhagya K Wijayawardena³; Michael P Kowalski²; Miranda Khermand Khermand²; Jennifer E Van Eyk¹; ¹Cedars Sinai Medical Center, Los Angeles, CA; ²University of Texas at Austin, Austin, TX; ³SLAC National Accelerator Laboratory, Standford, California

#### MP 288
**Bond Dissociation Calculations to Evaluate Molecular Fragmentation Caused by Hypervelocity Impacts in Closed-Source Mass Spectrometers**

Brandon Turner¹; Daniel E. Austin¹; Eric T. Sevy¹; ¹Brigham Young University, Provo, UT

#### MP 289
**New sample delivery and automation methods enable microsecond measurements in the X-ray footprinting mass spectrometry experiment**

Sayan Gupta¹; Line Kristensen²; Daniel P Deponte³; Matthew Rosi³; Brandon Russell³; Erik Farquhar³; Michael Sullivan³; Donald Abel³; Rohit Jain³; Shawn Costello³; Yan Chen³; Mark R. Chance³; Christopher J. Petzold³; Farid Farahmand⁴; Corie Y Ralston⁴; ¹Lawrence Berkeley National Laboratory, Berkeley, California; ²Lawrence Berkeley Laboratory, University of California, Berkeley, California; ³SLAC National Accelerator Laboratory, Standford, California; ⁴Sonoma State University, Rohnert Park, California; ²Brookhaven National Laboratory, Upton, NY; ⁴Case Western Reserve University, Cleveland, OH; ²University of California, Berkeley, CA; ⁴Lawrence Berkeley National Laboratory, Berkeley; ²Lawrence Berkeley National Laboratory, Berkeley, CA

#### MP 290
**Glow Flow: a step towards a universal ion source**

Rhodri N. Owen¹; Steve L Kelly¹; Gareth Brenton¹; ¹Swansea University, Swansea, United Kingdom
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**ION MOBILITY: FAIMS/DMS**

**MP 291-295**

**Low-Field Differential Ion Mobility Spectrometry of Dipole-Aligned Macromolecules**; Pratima Pathak¹; Alexandre Shvartsburg¹; ¹Wichita State University, Wichita, KS

**Distinguishing Unique Conformers of Monosaccharides using Differential Ion Mobility Spectrometry-Mass Spectrometry (DIMS-MS)**; Tiffany L Crawford¹; Gary L Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC

**Pre-filtration and separation of isomer pairs using Differential mobility spectrometry-mass spectrometry (DMS-MS)**; Ifeoluwa Ayodeji¹; Linxia Song²; Kenyon Evans-Nguyen²; Theresa Evans-Nguyen²; ¹University of South Florida, Tampa, FL; ²University of South Florida, Tampa, FL

**Proteomic analysis and isobaric separation using FAIMS interfaced mass spectrometry**; Laxmi Sinduri Vuppala¹; Theresa Evans-Nguyen¹; Petra Mick¹; Mahitha Nuthulaganti¹; ¹University of South Florida, Tampa, FL

**Protonation isomers of highly charged protein ions can be separated in FAIMS-MS**; J. Diana Zhang¹; Micah T. Dono²; Amber D. Rolland²; James S. Prell²; William A. Donald¹; ¹University of New South Wales, Sydney, Australia; ²University of Oregon, Oregon, Oregon

**ION MOBILITY: FUNDAMENTALS**

**MP 296-309**

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

**Effect of acetonitrile vapor in the ESI source on protomer distribution of protonated para-aminobenzoic acid (PABA)**; Zhaoyu Zheng¹; Athula B. Attygalle²; ¹Stevens Institute of Technology, Jersey City, NJ; ²Stevens Institute of Technology, Hoboken, NJ

**Collision Cross Section Calibration Strategies for a Prototype SLIM-based Ion Mobility Instrument**; Bailey S. Rose¹; Katrina L. Leaptrot¹; Kelly L. Wormwood Moser¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN; ²Mobilion Systems, Inc., Chadds Ford, PA

**Investigations on the formation of positive and negative reactant ions in High Kinetic Energy Ion Mobility Spectrometry (HIKE-IMS) by HIKE-IMS-MS**; Maria Allers¹; Duygu Ergoddu¹; Robin Hillen²; Walter Wissdorf²; Thorsten Benter²; Stefan Zimmermann²; ¹Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany; ²University of Wuppertal, Wuppertal, Germany

**Chemical Reaction and Transport Simulations of Positive Reactant Ions in High Kinetic Energy IMS (HIKE-IMS)**; Duygu Ergoddu¹; Maria Allers²; Walter Wissdorf²; Clara Markert¹; Hendrik Kersten¹; Stefan Zimmermann²; Thorsten Benter²; ¹University of Wuppertal, Wuppertal, Germany; ²Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany

**PhaseCRAFTI: a New Approach to Collision Cross Section Measurements Using FTICR/MS Phase Shifts**; David V. Dearden¹; Matthew C. Asplund³; Andrew J. Arslanian¹; Tina H. M. Farzan¹; Jamir Shrestha¹; ¹Brigham Young University, Provo, UT

**Compact HIKE-IMS for Quantitative Trace Gas Detection in Field Applications**; Florian Schlottmann¹; Ansgar T. Kirk¹; Alexander Bohnhorst¹; Maria Allers¹; Christoph Schaefer¹; Sebastian Kehlenbeck¹; Alexander Schwarz¹; Bert Ungethum¹; Falko Ziegert-Kuehni¹; Andreas Walte¹; Stefan Zimmermann¹; ¹Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Hannover, Germany; ²AIRSENSE Analytics GmbH, Schwerin, Germany

**Tandem DT-IMS/TIMS-MS for Accurate Mobility Measurements**; Kim Q Dang¹; Francisco Fernandez-Lima²; ¹FIU, Miami, FL; ²Florida International University, Miami, Florida

**Accurate Modeling of Peak Shapes and Drift Times in SLIM Traveling Wave Ion Mobility Spectrometry**; Sidney E. Buttrill, Jr.¹; Daniel Debord²; Liulin Deng²; ¹Consultant, Palo Alto, CA; ²MOBILion Systems Inc., Chadds Ford, PA

**Optimization of tristate gating and multiplexing parameters for improved ion mobility mass spectrometry of biomolecules**; Jim Butalez¹; James D. Sanders¹; Virginia K. James¹; Brian H Clowers²; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Washington State University, Pullman, WA

**Identifying the role of proton transfer reactions for proteins in the gas phase**; Tyler C Cropley¹; Mengqi Chai¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL

**Investigation of Resveratrol Photoisomerization Product by Ultra-Performance Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry (UPLC-IMS-MS)**; Gabriella V Litterio¹; Sihang Xu¹; Athula B. Attygalle¹; ¹Stevens Institute of Technology, Hoboken, NJ
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MP 308  Propagating error associated with TWIMS calibrations increases the accuracy of calculated CCS values; Alexis N. Edwards1; Hien M. Tran1; Elyssia S. Gallagher1; 1Baylor 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 Andaluz1; Viraj Gandhi1, 2; 1IUPUI, Indianapolis, IN; 2Purdue University, West Lafayette, IN

ISOTOPIC LABELLING AND FLUXOMICS APPLICATIONS
MP 310-314

MP 310  Hypothesis driven computational analysis of isotope tracer studies; Ethan Stancliffe1, 2; Michaela Schwaiger-Haber1; Miriam Sindelar1; Gary J. Patti1, 2; 1Department of Chemistry, Washington University in St. Louis, St. Louis, MO; 2Department of Medicine, Washington University in St. Louis, St. Louis, MO

MP 311  Cancer detection using 13C tracing and liquid biopsy; Likun Duan1; Grace Scheidemantle1; Xiaojing Liu1; 1North Carolina State University, Raleigh, NC

MP 312  DiLeuPMP: a multiplexed isobaric labeling method for high-throughput quantitative analysis of O-glycans; Ting-Jia Gu1; Miyang Li2; Lingjun Li1, 2; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706

MP 314  Integrating MetaboScape and PollyTM for the analysis of LC-TIMS-MS and LC-MS based fluxomics; Heino M. Heyman1; Heiko Neuweger2; Pawel Konrad Lorkiewicz2; Bradford G. Hill3; Kyle Fulghum3; Shefali Lathwal4; Avijit Zutshi5; Brian Dranka6; Swetabh Pathak3; Bradford G. Hill3; Kyle Fulghum3; Shefali Lathwal4; Avijit Zutshi5; Brian Dranka6; 1Bruker Scientific LLC, Billerica, MA; 2Bruker Daltonik GmbH, Bremen, Germany; 3University of Louisville, Louisville, KY; 4Elucidata, New Delhi, India; 5Elucidata, Delhi, India; 6Elucidata, Cambridge, MA

LC/MS: GENERAL
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MP 315  Development of a LC-MS/MS method for simultaneously determination of 30 pesticides in Chenpi; Xin Zheng1; Yueqi Li1; Taohong Huang2; 1Shimadzu(China) Co., LTD. Beijing Branch, Beijing, China; 2Shimadzu (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 Mull; 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 Larraillet1; Björn Mautz1; Maximiliane Koenig1; Michael Molhoj1; 1Roche Pharma Research and Early Development, Roche Innovation Center Munich, Germany

MP 318  Trace analysis of abused drugs in waste water sample by AOE system coupled with LCMS-8060; Jiaqi Liu1; Yunzhong Zheng1; Qisheng Zhong1; Taohong Huang2; 1Shimadzu (China) Co., LTD. Guangzhou Branch, Guangzhou, China; 2Shimadzu (China) Co., Ltd., Shanghai Office, Shanghai, China

MP 319  Transferring metabolomics methods from high-resolution Orbitrap to triple quadrupole mass spectrometers; Michaela Schwaiger-Haber1; Ethan Stancliffe1, 2; Miriam Sindelar1; Gary J. Patti1, 2; 1Department of Chemistry, Washington University in St. Louis, St. Louis, MO; 2Department 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-Ovanesyan1; Ling Xu1; David H Lee1; 1Mersana Therapeutics, Cambridge, MA

MP 322  LC/MS analysis of phosphonothioate 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 Yilmaz1; Abdulselam Ertas1; Oguz Cakir1; Ismail Yener1; Hamdi Temel1; 1Dicle University, Diyarbakir, Turkey

MP 326  Decellularized Extracellular Matrix Components Drive Cardiac Fate: Cues from Matrisome Influence Atrial Differentiation; Fernanda C P Mesquita1; Po-Feng Lee1; Yutao Xi1; Jacquelynn Morrissey1; Helen Andersson1; Gustavo Monnerat2; Fabio CS Nogueira2; Gilberto Domont2; Luiz C Sampaio2; Camila Hochman-Mendez2; Doris A Taylor1; 1Texas Heart Institute, Houston, TX; 2Federal University of Rio de Janeiro, Rio de Janeiro, Brazil
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

MP 327 Development of a sensitive LC-MS/MS Method for the Quantification of a Stereorepugnate Phosphorothioate Antisense Oligonucleotide in Human Plasma; Andrew Hart1; Susovan Mohapatra1; Esme Candish2; Ji Jiang3; 1Wave Life Sciences, Lexington, MA; 2Sciex, Framingham, MA

MP 328 Trace-level quantitative analysis of Poloxamers in biological samples by HPLC-ESI-QqQ MS; Ali Najafi1; Neelanjani Bose1; 1Emery Pharma, Alameda, CA

MP 329 Simplified high-throughput methods for deep and targeted proteome analysis on theimsTOFPro; Jarrod J Sandow1,2,3; Giuseppe Infusini1,2,3; Michael Krawitzky4; Christopher Adams4; Laura Dagley1,2; Rune Larsen1,2; Andrew I Webb1,2,3; 1The Walter & Eliza Hall Institute, Parkville, Australia; 2University of Melbourne, Parkville, Australia; 3IonOpticks, Fitzroy, Australia; 4Bruker Daltonics, San Jose, CA

MP 330 Effect of Vancomycin on Cytoplasmic Peptidoglycan Intermediate Levels In Resistant Enterococcus faecium; Shivani Gargvanshi; 1University 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; Jian-lin Wu1; Na Li2; 1Macau University of Science and Technology, Macau, Macau; 2Macau University of Science and Technology, Macao, Macao

MP 332 Expanding the versatility of the Eversep One with a toolbox of specialized workflows for MS-based omics; Dorte B. Bekker-Jensen1; Ole B. Horning1; Andreas-David Brunner2; Catherine G. Vasilopoulou2; Florian Meier2; Philipp E. Geyer2; Peter A. Nielsen1; Lasse Falkenby1; Jesper V. Olsen1; Ole Vorm1; Matthias Mann2; Nicolai Bache1; 1Eversep Biosystems, Odense, Denmark; 2Max Planck Institute of Biochemistry, Martinsried, Germany; 3Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

MP 333 Automating the Preparation of Matrix Matched Calibration Standards for the Analysis of Food Contaminants by LC/MS/MS; Fred Foster1; John Stuff1; Laurel Vernarelli1; Jacqueline Whitecavage1; 1Gerstel, Inc., Linthicum, MD

MP 334 Evaluation of sample preparation workflows for proteomics analysis of Chlamydomonas reinhardtii; Shin-Cheng Tzeng1; Ningning Zhang1; Ru Zhang1; Bradley Evans1; 1Donald Danforth Plant Science Center, Saint Louis, MO

MP 335 Steroid Screening in Horse Plasma via 96-Well Plate Supported Liquid Extraction; Deidre E. Damon1; Mohamed Youssef2; 1Ohio Department of Agriculture, Reynoldsburg, OH; 2Biotage, Charlotte, North Carolina

MP 336 Evaluation of trypsin activity through accelerated protein digestion at elevated temperatures; Alan A. Doucette1; Jessica Nickerson1; 1Dalhousie University, Halifax, NS

MP 337 Time and Money Savings by the Implementation of Automated µSPE for Cleanup of QuEChERS Extracts of Veterinary Drugs; Jonathan Beck1; Tom Plug1; Laura E Burns2; Dwayne E Schrunk2; Dipankar Ghosh3; Ed George3; 1CTC Analytics AG, Lake Elmo, MN; 2Iowa State University, Ames, IA; 3Thermo 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; Sami Bayoudh1; Mohamed Amine Ben Mlouka2; Pascal Cossette3; Julie Hardourn2; Kaynoush Naraghi1; Corentin Germann1; Michel Arotcarena1; 1AFFINISEP, Petit Couronne, France; 2PISSARO 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; Lee Williams1; Geoff Davies1; Katie-Jo Teehan1; Adam Senior1; Alan Edgington1; Helen Lodder1; 1Biologe GB Limited, Cardiff, United Kingdom

MP 341 Use of immobilized trypsin in proteomic workflows enables full automation and reduces undesirable by-products; Patrick Kates1; B. Todd Mullis2; Michael Walla2; William Cotham3; Qian Wang2; L. Andrew Lee1; 1Integrated Micro-chromatography Systems, Inc, Irmo, SC; 2University 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; Michae G. Ma1; Kelem Kassahun2; Rostislav Kuskovsky3; Yong Q. Tang1; Caroline A. Lee1; John S. Grundy1; 1Arena Pharmaceuticals, San Diego, CA; 2Frontage Laboratories, Inc., Exton, PA

MP 343 EasyPep Sample Preparation Technology for Rapid and Efficient Mass Spectrometry-based Proteomics; Sergei Snovida1; Amareeet Flora1; Bhabin Patel2; Penny Jensen2; Ryan Bomgarden2; 1Thermo Fisher Scientific, Rockford, IL; 2ThermoFisher Scientific, Rockford, IL

MP 344 Determination of Zoledronic Acid in Dog Serum by LC-MS/MS Xiaohua Li, Allan Xu1, 1Keystone Bioanalytical, Inc.; Allan Xu; Keystone Bioanalytical, North Wales, PA
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

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 Addink1; Tom Hall1; 1Fluid 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 Goldstein1; Pei Li1; Brendon E. Cook1; 1Biogen, Cambridge, MA

MP 347 Si-Trap: simultaneous, high throughput multilomics sample preparation; John Wilson1; Alexandre Zougman2; Lee D. Roberts3; Rosamonde E. Banks2; 1ProtiFi, LLC, Huntington, NY; 2University of Leeds, Leeds, United Kingdom; 3Leeds 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. Nikkii Sitasuwan1; Thomas W. Powers2; Tiffany Medwed2; Yuco Ogata3; Nancy S Nightlinger3; Richard S Rogers4; Casey Snodgrass5; Pamela Quizon1; L. Andrew Lee1; 1Integrated Micro-chromatography Systems, Inc, Irmo, SC; 2Pfizer Inc., Chesterfield, MO; 3Just - Evotec Biologics, Seattle, WA; 4Bristol-Myers Squibb, Seattle, Washington; 5Hamilton 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 Langille1; Fereshteh Shahhoseini1; Ali Azizi1; Christina Bottaro1; 1Memorial 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 Jashnani1; Srikanth Kotapati1; Jason Hogan1; Gavin Dollinger1; 1Bristol-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 Azizi1; Fereshteh Shahhoseini1; Evan Langille1; Christina Bottaro1; 1Memorial University, St. John’s, NL

LIPIDS: GENERAL

MP 352 Integrating Hydrophilic Interaction Chromatography, Trapped Ion Mobility Spectrometry, and Isomer Resolving MS/MS for In-Depth Lipidomic Profiling; Tian Xia1; Hengxue Shi1; Yu Xia1; 1Tsinghua University, Beijing, China

MP 353 Effect of Leishmania donovani infection on the lipidome and metabolome of RAW264.7 macrophage-derived exosomes; Andrew P Kurland1; Anna Gioseffi1; Peter Kima1; Timothy J Garrett1; 1University 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. Palagama1; Brock A Humphries1; Jagadish Boppisetti1; Youngsoo Jang1; Brian D Ross1; Gary D Luker1; 1University 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 Pannuk1; Nicole A. S.-Y. Dorville2; Yvonne A. Dzal2; Quinn E. Fletcher2; Kaleigh J.O. Norquay2; Craig K.R. Willis2; Albert J. Fornace Jr.1; Evagelia C. Laiakis1; 1Georgetown University Medical Center, Washington, DC; 2University of Wisconsin, Madison, WI

MP 356 Enhancement of lipid separation for the accurate quantification in nUHPLC-ESI-MS/MS; Jong Cheol Lee1; Myeong Hee Moon1; 1Department 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; Sergio P. Patii1; Grace M Jones1; Angela C Arata1; Russell Caccavello1; Krishna K Barakoti1; Ewan F Sinclair1; Alejandro Gugliucci1; Jean-Marc Schwarz1,2; 1Touro University California, Vallejo, CA; 2University of California San Francisco, San Francisco, CA

MP 358 Investigation of the altered brain myelin lipidome in the neurodegenerative disorder, Niemann-Pick Type C1; Chambinal Pathmasiri1; Melissa R. Pergande1; Fernando Tobias2; Stephanie M. Cologna1; Ernesto Bongarzone1; 1University of Illinois at Chicago, Chicago, IL; 2The Ohio State University, Columbus, OH

MP 359 Evaluation of the viability of HilIC- and RP-LC-HRMS and lipiddomics informatics for the characterization of strain-resolved Pseudomonas putida lipidomes; David T. Reeves1,2; William R. Henson2; Gregg T. Beckham2; Robert L. Hettich1,2; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Tennessee Knoxville, Knoxville, TN; 3National Renewable Energy Laboratory, Golden, CO

MP 360 Elucidation of Lipid Markers Associated with Smoke Inhalation Injury Using Multidimensional Skyline Lipid Spectral Libraries; Kaylie I Kirkwood1; Brian S. Pratt1; Kaipo Tamura1; Nicholas Shulman2; Sally Littau2; Amol M. Patwardhan1; Michael L. Heien1; Karen J. Richey2; Kevin N. Foster1; Jeffery L. Burgess3; Michael J. MacCoss2; Brendan X. Maclean2; Erin S. Baker1; 1Department of Chemistry, North Carolina State University, Raleigh, NC;
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

2Department of Genome Sciences, University of Washington, Seattle, WA; 2Zuckerman College of Public Health, University of Arizona, Tuscon, AZ; 4College of Medicine, University of Arizona, Tuscon, AZ; 3Department of Chemistry and Biochemistry, University of Arizona, Tuscon, AZ; 5The Arizona Burn Center, Maricopa Integrated Health Systems, Phoenix, AZ

MP 361 Role of neutral ceramidase in the pathogenesis of Alzheimer’s Disease; Farzana Parveen1; Vineet Kumar Mishra1; Shi Hui Law1; Hua-Chen Chan1; Liang-Yin Ke1; 1Kaohsiung Medical University, Kaohsiung City, Taiwan; 2Kaohsiung Medical University Hospital, Kaohsiung, Taiwan

MP 362 Resolving the anti-ferroptotic role of Nitric Oxide: Inhibiting 15LO/PEBP1 complex-mediated phospholipid peroxidation; Tamil Selvan Anthonyanuthu1; Indira H Shrivastava2; Anastasia Levkina3; Georgiy Vladimirov4; Zachary E Hier2; Andrew Amoscato2; Valerian E. Kagan5; Hulya Bayr6; 1University Of Pittsburgh, Pittsburgh, PA; 2University of Pittsburgh, Pittsburgh, PA; 3Laboratory 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 Valdebenito1; Brendan Prideaux2; Eliseo Eugenin2; 1University of Texas Medical Branch, GALVESTON, TX; 2University of Texas Medical Branch at Galveston, Galveston, TX

MP 364 A new method for the quantification of free fatty acids from disease state tissues; Peter M Lococo1; Madeline Colley2; Kenneth M Hargreaves3; Stephen Bach4; 1UTHSCSA, San Antonio, TX; 2University of Texas at San Antonio, San Antonio, TX; 3UTHSCSC, San Antonio

MP 365 A Complete Solution for Lipidomic Profiling of Bladder Cancer Patients using a Compact LC-oa-TOF; Lisa Reid1; Emmanuelle Claude1; Adam M King1; Gordon Fujimoto2; Robert Plumb3; Lauren Mullin4; 1Waters Corporation, Wilmslow, UK; 2Waters Corporation, Milford, MA

MP 366 A Rapid HILIC-IM-MSE Method and Structure Database for Bacterial Lipidomics; Christian Freeman1; Elijah Robert1; Kingsley Bimpeh1; Tabitha Lowe1; Shane Vahjen1; Keerthi Appala1; Kelly M Hines1; 1University of Georgia, Athens, GA

MALDI: APPLICATIONS

MP 368 Lipidomic changes and ethylidip phiacy associated with ether lipid deficiency in germinal centers of spleen: A multimodal IMS approach; Marissa Jones1, 2; Sung Hoon Cho3; Nathan Heath Patterson1, 2; Raf Van De Plas5; Clay F. Semenovkovich6, 7, 8; Mark R. Boothby9, 10, 11, 12; Jeffrey M. Spraggings1, 2, 4; Richard M. Caprioli1, 2, 4, 9, 12; 1Mass Spectrometry Research Center, Nashville, TN; 2Department of Chemistry, Vanderbilt University, Nashville, TN; 3Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; 4Department of Biochemistry, Vanderbilt University, Nashville, TN; 5Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; 6Division of Endocrinology, Metabolism & Lipid Research, Washington University School of Medicine, Saint Louis, MO; 7Division of Biology and Biomedical Sciences, Washington University School of Medicine, Saint Louis, MO; 8Department of Cell biology and Physiology, Washington University School of Medicine, Saint Louis, MO; 9Department of Medicine, Vanderbilt University, Nashville, TN; 10Department of Cancer Biology, Vanderbilt University, Nashville, TN; 11Vanderbilt-Ingram Cancer Center, Vanderbilt University, Nashville, TN; 12Department of Pharmacology, Vanderbilt University, Nashville, TN

MP 369 Multi-omic MS(IMS) analysis and identification of bacteria using liquid atmospheric pressure (AP) MALDI; Sophie Lellman1; Rainer Cramer1; 1University 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 Tominaga1; Takeshi Kasama1; Haruyuki Fijuno2; Shun Nokihara1; Atsushi Kitagawa1; Kiyoshi Nokihara1, 2; 1HiPep Laboratories, Kyoto, Japan; 2The First Affiliated Hospital with Nanjing Medical University, Nanjing, China

MP 371 Application of MALDI-MS for microcystin detection and imaging in mouse tissues; Daria Kucheravaia1; Nicholas J. Peraino2; Apurva Lad1; David J. Kennedy1; Steven T. Haller1; Judy A. Westrick2; Dragan Isailovic1; 1University of Toledo, Toledo, OH; 2Wayne State University, Detroit, MI

MP 372 Comprehensive pigment identification in Chlorella vulgarisby intact chloroplast MALDI-ET analysis; Luz A Calderón-Vergara1; Cristian Blanco-Tirado1; Marianny Y. Combariza-Montañez1; 1Universidad 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 Dikler1; 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 Chen1; He-Hsuan Hsiao1; 1Department of Chemistry, National Chung Hsing University, Taichung city, Taiwan
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MP 376  Fabrication of Antibody Decorated Boronic Acid Modified Gold Nanoparticles for the Rapid Diagnosis of Diabetes with LD1-TOF MS Analysis; Li-Sin Tu1; He-Hsuan Hsiao1; 1Department of Chemistry, National Chung Hsing University, Taichung city, Taiwan

MP 377  Changes in thymosin β4 during enteroïd generation demonstrated by direct MALDI-TOF-MS; Mohan Acharya1; Rohana Liyanage2; Jackson O Lay Jr. 2; Annie M Donoghue2; Narayan C Rath3; 1Department of Poultry Science, University of Arkansas, Fayetteville, Arkansas; 2University of Arkansas, Fayetteville, AR; 3USDA/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 Osta1; Pierre Naoubourg1; Bichr Alla2; Andreas Schnapp2; Tom K. Abban3; Shaunak Ibrahim4; Patrick Ducory5; 1Biomanoe, Dijon, France; 2Hôpital universitaire Robert-debré, Paris, France; 3Shimadzu Europa GmbH, Duisburg, Germany; 4Shimadzu, Manchester, UK, Manchester, United Kingdom

MP 379  Metastable Decomposition at the Peptide C-Terminal-Possible Use in Protein Identification;- Yang Wang1, 2; Etsuko Nakajima1; Yoshihito Okumura1; Danqing Wang1, 3; Nobuaki Okumura1; Toshifumi Takao1; 1Osaka University, Suita, Japan; 2Cedars-Sinai Medical Center, Los Angeles, CA; 3Fudan University, Shanghai, China

MP 380  High-Throughput Screening of Heavy Metal Ions with Peptide Decorated Gold Nanoparticles; Tzu-Hui Chiang1; He-Hsuan Hsiao1; 1Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan

MP 381  Imaging mass spectrometry in the analysis of lipids and metabolites for pancreatic tumors; Sina Feizbaksh Bazzargani1; Maria Guijarro Barrigon2; Richard A. Yost3; Maria Zajac-Kaye4; Timothy J. Garrett2; 1University of Florida, Gainesville, FL; 2University of Florida, Gainesville

MP 382  Mass spectrometry signatures of rabbit VX2 carcinoma model using MALDI imaging; Anna Colleen Crouch1; Dodge Lo Baluya1, 2; Emily A Thompson1; Elizabeth M Whitley1; Erik N.K. Cressman1; 1University of Texas MD Anderson Cancer Center, Houston, TX; 2Washington 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 Wu1; Renato Zenobi1; Pikyee Ma2; 1ETH Zurich, Zurich, Switzerland; 2Paul 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. Wood1; Sara K. Mattson1; Sylvia Stopka2; Gabor Maasz3; Zsolt Pirger3; Akos Vertes1; 1Department of Chemistry, The George Washington University, Washington, DC; 2Brigham and Women’s Hospital, Harvard Medical School, Boston, MA; 3Department 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 Shirato1; Kennesuke Hoshina1; 1Niigata 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 Hartmane1; Henriette Krenkel1; Michael Morris2; Rainer Cramer1; 1University of Reading, Reading, United Kingdom; 2Waters 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 Nicolardi1; David P. A. Kilgour2; Natasja Dolezal3; Jan W. Drijfhout3; Manfred Wuhrer1; Yuri E. M. Van Der Burgt1; 1Department of Proteomics and Metabolomics, LUMC, Leiden, Netherlands; 2Department of Chemistry, Nottingham Trent University, Nottingham, United Kingdom; 3Department 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 Moskovets1; Jace W. Jones2; Konstantin Novoselov1; Vladimir Doroshenko1; 1Mass Tech, Inc., Columbia, MD; 2University 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 Tucker1; Matthias Herrmann1; Haidy Metwally1; Richard Oleschuk1; 1Queen’s University, Kingston, ON

MP 390  A simple device to ease, speed up, and standardise MALDI-TOF sample preparation; Nadine Perrot1; Olivier Dauwalder2; Cécile Paris3; Alexia Barbry3; Stephanie Labich3; Corinne Beaulieu2; Bruno Colin2; Frederic Foucault2; Philippe Wandels2; Victoria Girard1; Karen Pinkston1; Geraldine Durand1; Francois Vandenbossche1; Jean-Philippe
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Charrier\textsuperscript{3}; \textsuperscript{1}BIOMERIEUX, La Balme Les Grottes, France; \textsuperscript{2}Hospices Civils de Lyon (HCL), LYON, France; \\
\textsuperscript{3}BIOMERIEUX, Marcy L’etoile, France; \textsuperscript{4}Biomerieux Inc, Hazelwood, MO 63042
**METABOLOMICS: SAMPLE PREPARATION**

**MP 391**  
An Automated, Combined Workflow for Extracting Polar Metabolites and Lipids from Mammalian Cells; Genevieve Van De Bittner¹; Alex Apfelft; Thu T.A. Nguyen, Kristin B. Bernick, Brian P. Smart, Reid Brennen, Christine Miller, Steven Fischer, Laurakay Bruhn; Agilent Technologies, Santa Clara, CA; University of Illinois at Chicago, Chicago, IL

**MP 392**  
Determining Minimum Cell Count for High-Quality Metabolite Identification and Metabolome Coverage; Casey A. Chamberlain, Kevin Cho, Sarah Chiang, Sisi Zhang, Sisi Zhang, Miriam Sindelar, Steven R. Doonan, Gary J. Patti; Washington University in St. Louis, St. Louis, MO

**MP 393**  
Nanosecond Photochemical Reaction (nsPCR) for Enhanced Identification and Visualization of Metabolites; Yuan Liu, Congyu Li, Lingjun Li; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 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, Robert Ninnis, Christopher Bowen, David De Souza, Kannan Ragunathan, Wei Boon Hon, Edredia L. Tull, Andrew A. Gooley, Trajan Scientific and Medical, Melbourne, Australia; Bio21 Institute, The University of Melbourne, Parkville, Australia; Shimadzu Scientific Instruments, Rowville, Australia; 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 Engrren, Curt Pettersson, Mikael Hedeland; Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden

**MP 397**  
Rapid analysis of S-Adenosylmethionine (SAM) and S-Adenosylhomocysteine (SAH) isopeptides in stable isotope-resolved metabolomics (SIRM) using direct nanoelectrospray ultra-high-resolution mass spectrometry; Joongeon Yang, Teresa Fan, Andrew Lane, Richard Higashi; Center for Environmental & Systems Biochemistry, University of Kentucky, Lexington, KY; Department of Toxicology and Cancer Biology, University of Kentucky, Lexington, KY; 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, David T Reeves, Richard J Giannone; Robert L Hettich; Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; University of Tennessee, Knoxville, TN

**MP 399**  
Assessment of a Metabolomics Automated Sample Prep Platform for Low Volume Plasma Samples; Mark Sartain, Manuel Gomez, Genevieve Van De Bittner, Henry Shu; Agilent Technologies, Santa Clara, CA

**MP 400**  
Impact of microcentrifuge tube selection on metabolomic results and some suggestions for best practices; Ah Young Yoon, Sujatha Chilakala, Stella Somianì, Katie Miller, Heather Blackburn, Vijay Eedunari, Hai Hu, Jerry S.H. Lee, Jonathan E Katz; Lawrence J. Ellison Institute for Transformative Medicine of USC, LOS ANGELES, CA; Chan Soon-Shiong Institute of Molecular Medicine at Windber, Windber, Pennsylvania; 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**  
Fast and Sensitive Determination of Targeted Intracellular Metabolites in Biological Fluids Using HILIC Negative Electrospray-Mass Spectrometry; Lianqiao Bian, Chongshan Dai, Ruiliu Wu, Rui Kang, Daolin Tang; Shimadzu Center for advanced analytical chemistry, Arlington, Texas; 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; Ruting Li, Bo Wen, Praveen Kumar, Jeremy Felton, Amit Pai, Duxin Sun; University of Michigan, Ann Arbor, MI

**MP 403**  
Quantitative analysis of acylcarnitines including isomeric and isobaric forms in biological matrices; Meshehvor Thapa, Daniela D. Weber, Sepedeh Aminzadeh Gohari, Barbara Ustaszewski, Barbara Koller, Guido Dallmann, Therese Koal; Research Program for Receptor Biochemistry and Tumor Metabolism, Department of Pediatrics, Paracelsus Medical University, Salzburg, Austria; 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; Giuoshi Sun, Richard Williams, Richard G. Kibbey; 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, Simona G. Codreanu, Don E. Davis, Jr., Christina C. Marasco, Fiona E. Harrison, Stacy D.
Targeted Metabolite Quantitation by MRM in Cell Culture Media: Evaluating Methods to Streamline Metabolite Analysis to Guide Cell Line Development; 

Elisa Gorre1; Andrew D Mahan2; 1JOHNSON AND JOHNSON, Spring House, PA; 2Johnson and Johnson, Spring House, PA

Development of polar metabolite profiling method by supercritical fluid chromatography/tandem mass spectrometry; 

Yutaka Konya1; Yoshihiro Izumi2; Takeshi Bamba1; 1Kyushu University, Fukuoka, Japan; 2Kyushu University, Fukuoka, Japan

Quantification of Metabolites Using the UPLC/MS-based AbsoluteIDQ p180 Kit; 

Vasanta Putluri1; Arun Sreekumar1; Nagireddy Putluri1; 1Baylor College of Medicine, Houston, TX

Integrating metabolomics as an important tool in pharmaceutical and biopharmaceutical drug research, discovery and development: Application case studies; 

Dewakar Sangaraju1; Allan Jaechico1; Zijuan Lai1; Merhya Tran1; Xiaorong Liang1; Nadja Katheder1; Heinrich Jasper1; Mary Keir1; Jordan Mar1; Allyson Byrd1; Jonathan Maher1; Tanja Zabka1; Paula Katavolos1; Anh Nguyen Dang1; Robert Shawley1; Yao Shi2; Clay Williams2; Dennis Milanowski2; Rachel Caminiti2; 1Genentech Inc, South San Francisco, CA; 2Covance Laboratories Inc., Madison, WI

A rapid and high throughput method for LC-MS/MS based quantitative determination of indol-3-acetic acid and trans-Zeatin; 

Anish Kundu1; Khushboo Adlakha1,2; Divya Goyal1; Faraz Rashid2; Dipankar Malakar2; Jyothilakshmi Vadassery1; 1National Institute of Plant Genome Research, Aruna Asaf Ali Marg., New Delhi, India; 2SCiEX, 121, Udyog Vihar, Phase – IV, Gurgaon, Haryana, India

Ovarian Cancer Metabolomics: Targeted Microchip Capillary Electrophoresis-Mass Spectrometry to Track Disease Progression; 

Samyukta Sah1; Marcos Bouza Areces2; Eunyong Park3; Olga Kim1; Jaeyeon Kim1,4; Facundo Fernandez2; 1Georgia Tech, Atlanta, GA; 2School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia; 3Indiana University School of Medicine, Departments of Surgery, Biochemistry and Molecular Biology, Indianapolis, Indiana; 4Indiana University Melvin & Bren Simon Cancer Center, Indianapolis, IN

Quantitation of amino sugars in leaf litter by chemical derivatization - LC/MS; 

Jun Han1,2; Alexandra Klem3; Evan Dyson-Loewen1; Juncong Yang1; David Schibli1; David R. Goodlett4,5; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC; 2Division of Medical Sciences, University of Victoria, Victoria, BC; 3University of Waterloo, Waterloo, ON; 4University of Maryland School of Dentistry, Baltimore, MD; 5University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland

Potential of metabolite sums and ratios calculations for faster biological insights into targeted metabolomics data; 

Martin Buratti1; Barbara Ustaszewski1; Gordian Adam1; Fadi Abd1; Therese Koal1; 1BIOCRATES Life Sciences AG, Innsbruck, Austria

Wide-range metabolomic analysis of hydrophilic metabolites by next-generation ion chromatography high resolution tandem mass spectrometry; 

Masatomo Takahashi1; Yoshihiro Izumi1; Takahiro Suzuki1; Kohta Nakatani1; Kosuke Hata1; Kentaro Takahara2; Takeshi Bamba1; 1Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; 2Thermo Fisher Scientific, Yokohama, Japan

Derivatization Approaches for Endogenous Steroid Hormones in Human Urine Using High-Resolution LC-MS; 

Lancia N.F. Darville-Bowleg1; Jayden C Cline1; Carrie Rozmeski1; Yessica C Martinez1; Shannan Rich2; Kathleen M Egan1; Lusine Yaghjian2; John M Koomen1; 1Moffitt Cancer Center, Tampa, FL; 2University of Florida, Gainesville, FL

Measurement of methylated metabolites using liquid chromatography-mass spectrometry; 

Chandra Shekar R Ambati1; Nagireddy Putluri1,2; Arun Sreekumar1; 1Advanced Technology Core, Dan L. Duncan Cancer Center, Alkek Center for Molecular Discovery, Baylor College of Medicine, Houston, TX 77030; 2Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX 77030; 3Department of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX, USA, Houston, TX 77030

Screening and Quantitation of Amino Acid and other components in Spent Media; 

Vikrant Goel1; Ashish Paraganka1; Sunil Raut1; Swarnendu Kaviraj1; Saikat Banerjee1; 1Agilent Technologies, Gurgaon, India; 2Agilent Technologies, BENGALURU, India; 3Gennova Biopharmaceuticals Ltd, Pune, India; 4Agilent Technologies India Pvt Ltd, Hyderabad, India

SCIEX 6500+ ESI-MS/MS: Impact of Advanced Scanning sMRM Mode on Peak Quality in Broad-spectrum metabolomics; 

Atul S Rathore1; Preeti Chandra1; Monique C Santana1; Colin D Kay1; 1Food Bioprocessing & Nutrition Sciences, Plants for Human Health Institute, North Carolina State University, North Carolina Research Campus, 600 Laureate Way, Kannapolis, NC

Targeted metabolic analysis of tricarboxylic acid cycle intermediates and amino acids in human plasma following chemical derivatization; 

Adam Cseresnye1,2; Claire Jeanine Colette Huguernaud1,2,3; James E. Evans1,2; Michael Mullan1,2,4; Fiona Crawford1,2,4; Laila Abdullah1,2,4; 1Roskamp Institute, Sarasota, FL;

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2James A. Haley Veterans’ Hospital, Tampa, FL; 3Open University, Milton Keynes, United Kingdom; 4Open 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**; Takanari Hattori; Jun Watanabe; Junko Iida; Shimadzu Techno-Research, Inc., Kyoto, Japan; 2Shimadzu Corporation, Kyoto, Japan

**MP 422**

Multiplexed quantification of bile acids with LC-MS for characterization of mouse gut microbial metabolism; **Armando Alcazar Magana**; Yang Zhang; Adrian Gombar; Jan F. Stevens; Claudia Susanne Maier; Department of Chemistry, Oregon State University, Corvallis, OR; 2Linus Pauling Institute, Corvallis, Oregon; 3School of Biological and Population Health Sciences, Corvallis, Oregon; 4Department of Biochemistry and Biophysics, Oregon State University, Corvallis, Oregon; 5Department 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**; Hirotaka Kuroda; Takashi Suzuki; Toru Ezure; 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**; Nicole M. Davis; Zijie Xia; David S. Schneider; Allis S. Chien; Stanford University Mass Spectrometry, Stanford, CA; 2Dept. 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**; Daniele Simoneschi; Michele Pagano; Drew Jones; NYU Langone Health, New York, NY

**MICROORGANISMS AND THE MICROBIOME I**

**MP 426**

Accounting for chimeric spectra boosts the number of identifications in metaproteomics without impacting sensitivity; **Tim Van Den Bossche**; Thilo Muth; Lennart Martens; Viktoria Dorfer; VIB - UGent Center for Medical Biotechnology, Gent, Belgium; 2Science Division (S.3), Federal Institute for Materials Research and Testing, Berlin, Germany; 3Bioinformatics 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**; Odeta Qafoku; Kaitlyn Schwarz; Zhihua Zhu; Lindsey Anderson; Geremy Clair; William Nelson; Mark Engelhard; Mark Bowden; Janet Jansson; Kirsten Hofmockel; Christopher Anderton; 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**; Zeljko Dvnajsak; Galina Glazko; Yasir Rahmatallah; Alan Tackett; Lisa Orr; Samuel Mackintosh; John Arthur; Boris Zybyaylov; UAMS, Little Rock, AR; 2Arkana 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**; Xiaoxia Gong; Parvin Mirzaei; Rui Wang; Volker Neugebauer; Yehia Mechref; Chwani-Li Shen; Texas Tech University, Box 43132 Lubbock, TX; 2Texas 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**; Ashish Chakraborty; Lindsey Kirkpatrick; Rachel D Downey; Sarmistha B Hauger; Oleg Karaduta; Zeljko Dvnajsak; Galina Glazko; Yasir Rahmatallah; Alan Tackett; Lisa Orr; Samuel Mackintosh; John Arthur; Boris Zybyaylov; UAMS, Little Rock, AR; 2Arkana Laboratories, Little Rock, AR

**MP 431**

The Metabolic State Of Syndiotrophic Bacteria Effects Proteomic Acylation Profile; **John Muroski**; Hong H Nguyen; Michael J McNerney; Rachel RO Loo; Joseph A. Loo; University of California, Los Angeles, Los Angeles, CA; 2University of Oklahoma, Norman, OK

**MP 432**

Host diet directs structure and immunomodulatory capacity of gut symbiont-originated glycosphingolipids; **Sungwhan F Oh**; Jisun Yoo; Changwon C Lee; Deniz Erturk-Hasdemir; Hee Bum Song; Leda Gebremedhin; Seung Bum Park; Dennis L Kasper; Brigham and Women’s Hospital, Boston, MA; 2Harvard Medical School, Boston, MA; 3Seoul 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**; Ilaria Pertot; Gerardo Puopolo; Martina Marchetti-Deschmann; Fondazione Edmund Mach, San Michele all’Adige, Italy; 2University of Udine, Udine, Italy; 3University of Trento, San Michele all’Adige, Italy; 4TU Wien, Vienna, Austria

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Predicting metabolite production in gut microbes by integrating flux balance analysis with untargeted metabolomics; Erica Marie Forsberg1; Matt Manney2; Ellen Kuang2; Rob Edwards2; 1San Diego State University, San Diego, CA

Proteolytic Maturation and Copy Number Determination in a Giant SalmonellaVirus; Aaron Scheuch1; Sara Mallory2; Julia Farone2; Sammy Pardo3; Dana Moller4; Ru-ching Hsia5; Susan T. Weintraub6; Julie A. Thomas7; 1Rochester Institute of Technology, Rochester, NY 14623-5603; 2University of Texas Health Science Center at San Antonio, San Antonio, TX 78229-3900; 3University of Texas Health Science Center at San Antonio, San Antonio, TX 78229; 4University of Maryland School of Dentistry, Baltimore, MD 21201

Morphine administration, genetics, and high fat diet alters the mouse gut microbiome composition and function in lean and obese mice; Jose Alfredo Blakeley-Ruiz1,2; Carlee S. McClintock2,3; Him K Shrestha1,2; Suresh Poudel2; Richard J. Giannone2; Mircea Podar1,2; Helen A. Baghdoyan1,2; Richard J. Giannone2; 1University of Tennessee, Knoxville, TN; 2Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; 3Pain Consultants of East Tennessee, Knoxville, TN; 4University of Tennessee Knoxville, Knoxville, TN

Proteomic and metabolomic characterization of the syntrophic interactions between TM7 phylotype and Actinomyces odontolyticus; Fabian Schulte1,2; Batileg Bor1,2; Lujia Cen1; Pooja Balani1,2; Tsute Chen1; Markus Hardt1,2; Xuesong He1,2; 1Forsyth Institute, Cambridge, MA; 2Harvard School of Dental Medicine, Boston, MA

MiCIdGUI: A user friendly graphical interface for MiCld a tool for Microorganism Classification and Identification; Aleksey Ogurtsov1; Gelio Alves1; Yi-Kuo Yu1; 1National Center for Biotechnology Information, NLM, Bethesda, MD

LC-HRMS and GCxGC-TOFMS characterization of storage conditions for metabolite screening in human whole stool samples; Paulina Piotrowski1; Christina Jones2; 1National Institute of Standards and Technology, Gaithersburg, MD; 2National Institute of Standards and Technology, Gaithersburg, Maryland

A practical workflow for training in gut metaproteomics studies; Mona M. Khamis1; Xu Zhang1; Zhibin Ning1; Krystal Walker1; Leyuan Li1; Kai Cheng1; Janice Mayne1; Daniel Figeys1; 1Ottawa Institute of Systems Biology and Department of Biochemistry, Microbiology and Immunology, University of Ottawa, Ottawa, ON

The Archaeal Proteome Project – advancing knowledge about archaeal cell biology through comprehensive proteomics; Stefan Schulte1; Zachary Adams2; Micaela Cerletti3; Rosana De Castro4; Sébastien Ferreira-Cerca5; Christian Fufezan6; Maria Inês Giménez7; Michael Hippler8; Zivojin Jevtic9; Robert Knüppel10; Georgio Legerme11; 1University of Pennsylvania, Philadelphia, PA; 2University of Florida, Gainesville, FL; 3National University of Mar del Plata, Mar del Plata, Argentina; 4University of Regensburg, Regensburg, Germany; 5Heidelberg University, Heidelberg, Germany; 6University of Münster, Münster, Germany; 7Max Planck Institute for biophysical chemistry, Göttingen, Germany; 8Ulm University, Ulm, Germany; 9Ruhr University Bochum, Bochum, Germany

Liver Toxicity and Alteration of Renin-Angiotensin System (RAS) Components Induced by Silver Nanoparticle Exposure in Wistar Rats; Subhayu Nayek1; Imesha W. De Silva1; Amie K. Lund1; Guido F. Verbeck1; 1University of North Texas, Denton, TX

Characterization of Nanoparticles Embedded in Organic Matrices by Cluster-SIMS; Stanislav Verkhoutrov1; Nathan A. Fleer2; Dmitriy S. Verkhoutrov2; 1Texas A&M University, College Station, TX; 2Texas A&M, College Station, TX

Structure and dynamics of inorganic polymers in solution studied with high-resolution MS, LC/MS and 16O/18O exchange: focus on polyoxometalates; Daniel Favre1; Igor A Kaltashov1; 1Univ. of Massachusetts/Chemistry Dept., Amherst, MA

Quantitative LC-MS/MS Analysis of PEGylated and non-PEGylated Lipid Mixtures from Lanthanide Nanoparticle-Supported Lipid Bilayers; Loryn P. Arnett1; Matthew W Forbes1; Mitchell A. Winnik1; 1University of Toronto, Toronto, ON

Separation and detection method for polyphenols and its associated isomers using ion-mobility mass spectrometry; Iwao Sakane1; Hajime Mizuno2; Eiji Sugiyama2; Kentaro Takahara3; Reiko Kiyonami4; 1ITO-EN LTD, Tokyo, Japan; 2University of Shizuoka, Shizuoka, Japan; 3Thermo Fisher Scientific Japan, Tokyo, Japan; 4Thermo Fisher Scientific, San Jose, CA
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**MP 447** Analysis of Vitamin E acetate in Hemp vape oil products; Sue Dantonio¹; Robert A. Dantonio²; Nikolais Lau³; ¹Agilent Technologies, Cedar Creek, TX; ²Texas A & M University, Corpus Christi, Texas; ³Agilent Technologies, Chicago, IL

**MP 448** Structural moieties and tissue distribution of hepatoprotective lignin-derived agent determined by isotopic labeling mass spectrometry; Alexander Zherebker⁴; Oleg Kharybin⁵; Alexey Orlov⁶; Oxana Kovaleva⁷; Oliver J. Lechtenfeld⁸; Elena Fedoros⁹; Irina Perminova¹⁰; Eugene (evgeny) Nikolaev¹¹; ⁴Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; ⁵Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany; ⁶N.N. Petrov National Medical Research Center of Oncology, Saint-Petersburg, Russia; ⁷Lomonosov Moscow State University, Chemistry Department, Moscow, Russia; ⁸Skolkovo institute of science and technology, Moscow Region, Russian Federation

**MP 449** Discovery of Bioactive Proteins from Scorpion Venom using Two Dimensional Mass Spectrometry; Meng Li¹; Yoko Pui Yiu Lam²; Christopher A. Wootton³; Peng Chen⁴; Remy Gavard⁵; Cookson K. C. Chiu⁶; Bryan P. Marzullo⁷; Qiong Wu⁸; Tomes E. Morgan⁹; Mark P. Barrow⁴; Hongzheng Fu²; Peter B O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²Peking University, Haidian, China

**MP 450** Cyclic Peptide Tandem-MS Search Software; Marshall Bern¹; A. Michelle English¹; Wilfred Tang¹; Chia-Wei Chia-Wei Lin²; Hannelore Kaspar²; Emmanuel Matabaro²; Markus Künzler²; ¹Protein Metrics, Cupertino, CA; ²ETH Zurich, Zurich, Switzerland

**MP 451** Establishment and application of a natural product LC-MS/MS library for plant metabolomics; Wenbin Wu¹; Jeffrey Morrë²; Valtcho Jeliazkov³; Jett Guerra⁴; Jan F. Stevens⁵; ¹Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon 97331; ²Department of Chemistry, Oregon State University, Corvallis, Oregon 97331; ³Department of crop and soil science, Oregon state university, Corvallis, Oregon 97331; ⁴Department 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; Richard B. Van Bremen¹; Ruth N. Muchin²; Jaewoo Choi¹; Dana M. Gibbon¹; Brett Tyler¹; ¹Oregon State University, Corvallis, OR; ²Oregon State University, Corvallis, 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. Quizon¹; Michael Russelle S. Alvarez¹; Kimberly M. Delica¹; Manolo L. Basingan, Jr.¹; Froila Marie G. Deniega¹; Rowell P. Abogado²; Patrick Moreno³; Luster S. Labarga⁴; Mylene Ross P. Arcena¹; Isagani D. Padolina⁵; Francisco M. Heralde lii⁶; Gladys Cherisse J. Compele³; Ruel C. Nacario¹; ¹University of the Philippines Los Baños, Laguna, Philippines; ²Pascual Pharma Corp., Laguna, Philippines; ³Lung Center of the Philippines, Quezon City, Philippines

**PEPTIDES: PTM IDENTIFICATION I**

**MP 454** Multi-Level Post-Translational Modification Classification with PTM-Shepherd; Daniel J Geiszler¹; Dmitry Avtonomov¹; Andy Kong¹; Fengchao Yu¹; Felipe V Leprevost¹; Hui-Yin Chang¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI

**MP 455** Mass spectrometry-based precise identification of endogenous citrullinated histone in human astrocytoma U87 cells; Bin Wang¹; Yatao Shi¹; Zihui Li²; Xudong Shi²; Lingjun Li³; ¹School of pharmacy, University of Wisconsin-Madison, Madison, WI 53705; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; ³Department 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; Xiaolu Li¹; ²; Tong Zhang¹; Matthew J. Gaffrey¹; Ronald J. Moore³; Bin Yang³; Wei-Jun Qian¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Washington State University, Richland, WA

**MP 457** Disulfide bond and glycosylation site occupancy mapping of monoclonal antibodies using a novel capillary MAbPac column; Zoltan Szabo¹; Xuefei Sun²; Brandon H. Robson²; Lin Shanhua²; Dietmar Reusch³; Mike Bayham⁴; Rainer Bauder⁴; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, Sunnyvale, California; ³Roche Diagnostics GmbH, Penzberg, Germany; ⁴Thermo Fisher Scientific, Runcorn, United Kingdom; ⁵Thermo 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; Michael C Hare¹; Valery G. Voinov¹; ²; Yury V. Vasil'ev¹; ²; Joseph C. Meeuwsen¹; ²; Joseph S. Beckman¹; ²; ¹e-MSion Inc., Corvallis, Oregon; ²Oregon State University, Corvallis, OR

**MP 459** Characterization of Capsid Protein Post Translational Modifications Using High Resolution Mass Spectrometry; Sean McCarthy¹; Kerstin Pohl²; Esme Candish²; ¹SCIEX, Framingham, MA; ²Sciex, Framingham, MA

**MP 460** MS Characterization of Extensible Peptides From Cell Walls: Identification of Intra- and Intermolecular Cross-links and Abundance of Internal Fragment Ions; Lawrie Veale¹; Ankur Patel²; Steven D Hartson¹;
MP 461 Counterion Optimization Dramatically Improves Selectivity for Phosphopeptides and Glycopeptides in Electrostatic Repulsion-Hydrophilic Interaction Chromatography (ERLIC); Yusi Cui1; Dylan Nicholas T Tabang1; Zishan Zhang1; Min Ma1; Andrew J. Alpert1, 2; Lingjun Li1; 1University of Wisconsin-Madison, Madison, WI; 2PolyLC Inc., Columbia, MD

MP 462 Revealing dynamic protein acetylation across subcellular compartments; Alexis J Lawton1; Josue Baeza1; John Denu1; 1University of Wisconsin-Madison, Madison, Wisconsin

MP 463 Development of a novel mass spectrometry decision tree for O-GlcNAc site mapping; John W. Thompson1; Michael J. Sweredoski2; Matthew E. Griffin1; Brett Lomenick2; Annie Moradian1; Spirios D. Garbis2; Linda C. Hsieh-Wilson1; 1Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; 2Proteome 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; Nonko Fujii1; Takumi Takata1; Ingu Kim1; Toshiya Matsubara2; 1Institute for Integrated Radiation and Nuclear Science, Kyoto University, Sennan-gun, Japan; 2Shimadzu Corporation, Kyoto, Japan

MP 465 Complementarity of EThcD and HCD of Glycopeptides: Y ion Filtering for Increased Glycopeptide Identification; Robert Chalkley1; Katalin F Medzihradszky1, 2; Adam Pap2; Zsuzsanna Darula2; Peter R Baker1; 1University of California San Francisco, San Francisco, CA; 2Biological 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; Georges Bedran1; Marcos Yebenes1; Sachin Kote1; Irena Dapic1; Kamila Pawlicka2; Satya Saxena3; David Goodlett4; Robin Fahraeus5; Ted Hupp1, 2; Javier A Alfaro1, 2; 1University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland; 2University of Edinburgh, Edinburgh, United Kingdom; 3Deurion LLC, Seattle, WA; 4University of Maryland Baltimore, Baltimore, MD; 5INSERM, Paris, France

MP 467 Mass spectrometric quantification of histone lactylation marks in human melanoma cells; Kevin Huang1, 2; Ziyuan Li3; Lu Yang1; Jinjun Gao1; Di Zhang1; Yingming Zhao1; 1Ben May Department for Cancer Research, The University of Chicago, Chicago, Illinois; 2St. Mark’s School in Southborough, Massachusetts, MA; 3School of Pharmacy, University of Wisconsin-Madison, Madison, WI

MP 468 Polyubiquitin chain architecture detected by mass spectrometry; bo-shieng Hsu; National Taiwan Ocean University, Keelung, Taiwan

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS

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MP 469 Characterization of the nucleoporin complex Red8 by native mass spectrometry; Andrew Norris1; Brian Caldwell1; Charles Bell1; Vicki H. Wysocki1; 1The Ohio State University, Columbus, OH

MP 470 Collision Induced Dissociation of Higher-Order Hemoglobin Complexes Reveals Quaternary Structure Information; Alexander I.M. Sever1; Victor Yin1; Lars Konermann1; 1The 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; Nancy Wiebelhaus1; Jacqueline M. Zaengle-Barone1; Katherine J. Franz1; Michael C. Fitzgerald1; 1Duke University, Durham, NC

MP 472 Differential assembly of ERBB signaling complex provides mechanistic insight on kinase inhibitor sensitivity in cancer cells; Shujuan Wang1; Cunjie Zhang2; Xiaojing Wu1; Pan Zhang1; Qing Sheng2; Carl UlI Bialucha3, 4; Karen Colwill1; Yong Zheng1, 2; 1Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China; 2Lunenfeld Tanenbaum Research Institute, Toronto, M5G 1X5; 3Novartis Institutes for Biomedical Research, Cambridge, Massachusetts; 4University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland

MP 473 Native mass spectrometry analysis of the macromolecular organization of Get3-Get4-Get5 protein complex; Fabian Giska1; Malayalam Mariappan1; Kallol Gupta1; 1Nanobiology 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; Eva Illes-Toth1; James W. Hughes1; Helen J. Cooper1; 1University of Birmingham, Birmingham, United Kingdom

MP 475 How variable is your pore-forming protein toxin oligomeric state in different detergent environments; Amber D. Rolland1; Jesse W. Wilson1; Lejla S. Biberic1; James S. Prell1; 1University of Oregon, Eugene, OR
Check before you plunge: native MS as a diagnostic and screening platform in preparing macromolecular assemblies for cryo-EM analysis; Paul Dominic B. Olinares; James Chen; Courtney Chiu; Jin Young Kang; Eliza Lewellyn; Ruth Saecker; Elizabeth Campbell; Seth Darst; Brian T. Chat; The Rockefeller University, New York, NY; Korea Advanced Institute of Science and Technology, Daejeon, South Korea

Global Analysis of Surfaceome Interaction Network by Integrating Chemical Cross Linking and MS-based Proteomics; Fangxu Sun; Ronghu Wu; Georgia Tech, Atlanta, GA; Georgia Institute of Technology, Atlanta, GA

Characterization of high-mass multivalent antigen/antibody complexes by native ESI MS; Yang Yang; Igor A. Kaltashov; University of Massachusetts Amherst, Amherst, MA

Approaching a complete yeast interactome – combining a robust high-throughput pull-down workflow with fast and sensitive Evosep/timsTOF Pro analysis; André Clemens Michaelis; Andreas-David Brunner; Maximilian Zwiefel; Isabell Bludau; Maximilian T. Strauss; Florian Meier; Matthias Mann; Max Planck Institute of Biochemistry, Martinsried, Germany; Nordico Novo Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark

ATF4 Promotes Skeletal Muscle Atrophy by Forming a Heterodimer with CEBP; Scott M. Ebert; Jacob Rose; Steven A. Bullard; Nathan Basisty; George R. Marcotte; Birgit Schilling; Chris Adams; University of Iowa, College of Medicine, Iowa City, Iowa; Buck Institute, Novato, CA

Our first line of defense: Understanding the mechanism of a novel bactericidal protein using NativeMS; Anushka Halder; Kallol Gupta; Ryan Gaudet; John Macmicking; University of Maryland, College Park, MD; Northwest National Laboratory, Richland, WA; Agilent Technologies, Wilmington, DE

Investigation into the Mutations Associated with Mohr Syndrome Reveals a critical role for Integrator Proteins; William K Russell; Lauren G Mascibroda; Eric J Wagner; University of Texas Medical Branch, Galveston, TX

RNA Polymerase II Interactome Analysis for Characterization of Transcriptional Elongation Stress; Dominique A Baldwin; Katlyn D Hughes Burris; Jose F Victorino; Amber L Mosley; Indiana University School of Medicine, Indianapolis, IN; Indiana University School of Medicine, Indianapolis, IN

Platelet factor 4 interactions with heparin oligomers: implications for folding and assembly in vivo; Chendi Niu; Yang Yang; Igor A. Kaltashov; University of Massachusetts Amherst, Amherst, MA

Exposing the heterogeneity of the 20S proteasome by mass spectrometry; Gili Ben-Nissan; Shay Vimer; Zac Vanarrennum; Benjamin J. Jones; Dalton T. Snyder; Vicki H. Wysocki; Yury V. Vasil'ev; Joe S. Beckman; University of Massachusetts Amherst, Amherst, MA; Georgia Tech, Atlanta, GA; Pacific Northwest National Laboratory, Richland, WA

The Effect of Ionic Strength on Measured Metalloenzyme-Ligand Binding Constants in Native Mass Spectrometry; Taylor Perkins; Wonhyeung Jung; Rachel Ogorzalek Loo; Joseph A. Loo; University of California, Los Angeles, CA

Characterization of DNA Damage, Phosphorylation, and Domain-Specific Interactors of the p53 Transactivation Domains; Lisa M. Jenkins; Andres Thorkelson; Sudipto Das; Harichandra D. Tagad; University of Massachusetts Amherst, Amherst, MA

Hybrid mass spectrometry analysis of multimembrane-spanning efflux pump assemblies; Tarick J El-Baba; Jani Reddy Bolla; Francesco Fiorentino; Di Wu; Leonard Umer; University of Oxford, Oxford, United Kingdom

Native mass spectrometry and surface-induced dissociation reveal stabilization of Hfq:RNA complexes by intrinsically disordered C-terminal domain; Samantha H Sarn; Mengxuan Jia; Vicki H Wysocki; Ewelina Malecka-Grajek; Dorjehe Roca; Sarah Woodson; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Technical University of Munich, Munich, Germany; Resource for Native Mass Spectrometry; Guided Structural Biology, Columbus, OH; Ohio State Biochemistry Program, The Ohio State University, Columbus, OH; T. C. Jenkins Department of Biophysics, Johns Hopkins University, Baltimore, MD

Native MS of Protein Complexes: Application of a Next Generation Q-ToF Mass Spectrometer; Christopher Mallis; Xueyun Zheng; Xi Qiu; David H. Russell; Texas A&M University, College Station, TX; Agilent Technologies, Wilmington, DE
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

MP 492  Quantifying Membrane Protein-Lipid Interactions by Lipid Exchange-Mass Spectrometry; Guozo Zhang1; Hiruni Jayasekera1; James Keener1; Michael Thomas Marty1; 1University of Arizona, Tucson, AZ

MP 493  Proximity Ligation by Antibody Recognition for Interactome Studies; Shujiang Dai1; Juliane Weißer2; Bailin Zhang1; 1Sanofi, Cambridge, MA; 2Sanofi, Framingham, MA

MP 494  HDX-MS probes respiratory syncytial virus (RSV) antagonism of the host innate immune response; Nicole D. Wagner1; Jingjing Pei1; Angela Zou2; Gayaa K. Amarasingshe2; Michael L. Gross1; Daisy W. Leung2; 1Washington University School of Medicine, St. Louis, MO; 2Washington 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

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MP 496  Novel Proteomic Approaches to Characterize Endogenous Integral Membrane Protein; Kyle Brown1; Christian Eken1; Trisha Tucholski1; Song Jin1; Ying Ge1; 1University of Wisconsin, Madison, WI

MP 497  Development of lysosome membrane and membrane-binding proteomic strategies both in vitro and in vivo; Saadia Hasan1; Ashley Frankenfield2; Michael Ward1; Ling Hao2; 1National Institute of Neurological Disorders and Stroke, Bethesda, MD; 2George 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. Chu1; Patrick D. Perkins1; Christian Klein1; 1Agilent 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 Suttapitugsakul1; Ming Tong1; Ronghu Wu1; 1Georgia Institute of Technology, Atlanta, GA

MP 501  Establishing proteoliposomes for the analysis of membrane proteins by mass spectrometry; Melissa Frick1; Julian Bender1; Carla Schmidt1; 1Interdisciplinary 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) Xie1; Ying Sheng1; Qiongyu Li1; Seunghye Ju1; Joe Reyes2; Carlito B Lebrilla1; 1University of California, Davis, Davis, CA; 2University 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 Luceck1; Matthew Waas2; Rebekah L. Gundry1; 1Department of Biochemistry, Medical College of Wisconsin, Milwaukee, WI, 53226; 2CardioML 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. Verkhoturov1; Michael J. Eller2; Yong Duk Han3; Stanislav V. Verkhoturov4; Alexander Revzin2; Emile A. Schweikert1; 1Texas A&M, College Station, TX; 2California State University Northridge, Northridge, CA; 3Mayo Clinic, Rochester, MN

MP 505  G protein-coupled receptor (GPCR)-interacting proteins probed by chemical cross-linking and mass spectrometry; Bill Huang1; Hee-yong Kim1; 1NIAAA/NIH, Rockville, MD

MP 506  De Novo Peptide Sequencing from Mass Spectrometry Data with Deep Learning; Michelle Gill1; Joyjit Daw1; Johnny Israeli2; 1NVIDIA, New York, NY; 2NVIDIA, Santa Clara, CA

MP 507  Hydrogen-deuterium Exchange MS elucidates mechanotransmission mechanism of the MacB ABC transporter; Kjetil Hansen1; Nick Greene2; Vassilis Koronakis2; Argyris Politis1; 1King's College London, London, United Kingdom; 2University of Cambridge, Cambridge, United Kingdom

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MP 509  Viral-mediated ubiquitination impacts interactions of host proteins with viral RNA and promotes viral RNA processing; Christin Hermann1; 2; Jennifer C. Liddle1; 2; Joseph M. Dybas1; 2; Alexander M. Price1; 2; Matthew Charman1; 2; Eui Tae Kim1; 2; Richard Lauman1; Benjamin A. Garcia2; Matthew D. Weitzman1; 2; 1Div. of Protective Immunity and Div. of Cancer Pathobiology, Children's Hospital of Philadelphia, Philadelphia, PA; 2Dept. 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 Li1; Yatao Shi2; Bin Wang3; Lingjun Li2; 1University of Wisconsin Madison, Madison, WI; 2University of Wisconsin-Madison, Madison, Wisconsin

MP 511  Hydrophilic enhanced dual-functionalized Titanium (IV) IMAC material for enrichment and separation of glycopeptides and phosphopeptides; Danqing Wang1; Junfeng Huang2; Min Ma2; Lingjun Li1; 2; 1Department of
MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

Chemistry, University of Wisconsin-Madison, Madison, WI 53706; 2School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705

MP 512 Evaluation of enrichment strategies for confident identification of prenylated proteins; Zixiang Fang1; Saiful M. Chowdhury1; 1University of Texas Arlington, Arlington

MP 513 Ubiquitination promotes protective response to DNA-protein crosslinks; Luke Erber1; Natalia Tretyakova1; 1University 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 Bade1; Lin Li2; Kailin Yu1; Xiaoxia Dai1; Weili Miao1; Yinsheng Wang1; 1UC Riverside, Riverside, CA; 2UC RIVERSIDE, Riverside, CA

MP 515 Isomers and Fibrils: Wrenches in the Gears of Lysosomal Digestion; Tyler R Lambeth1; Ryan R. Julian2; 1University of California-Riverside, Riverside, CA; 2University of California, Riverside, Riverside, CA

MP 516 Phosphoproteome Quantification by TMT and DIA; Billy W Newton1; Yi Zeng1; Jia Tang1; Guanghui Han1; 1BGI 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 Mann1; Yanlong Zhu2; Eil Larson1; Ying Ge1; Allan R Brasier1; 1University of Wisconsin-Madison, Madison, Wisconsin; 2University 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 Sun1,2; Ruchika Bhawal3; Hui Xu1; Elizabeth Anderson3; Sheng Zhang3; Gary Gibson1; 1Weill Cornell Medicine, New York, NY; 2College of Medicine, Jiaxing University, 314001, China, Jiaxing, China; 3Cornell University, Ithaca, NY

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MP 521 Comparing an intrinsically disordered protein α-synuclein to fixed structure proteins following FPOP modification using high resolution LCMS intact analysis; Alan Barnes1; Jake A Busutilt-Goodfellow2; James Ault2; Neil J Loftus1; Frank Sobott1; 1Shimadzu MS/BU, Manchester, United Kingdom; 2University of Leeds, Leeds, United Kingdom

MP 522 Unravelling hundreds of proteoforms of heavily glycosylated enzymes using native-like LC-MS analysis; Michiel Akeroyd1; Olaf Schouten1; Stephane Bahraoui2; Marshall Bern2; 1DSM Biotechnology Center, Delft, Netherlands; 2Protein Metrics Inc, Cupertino, CA

MP 523 Capillary chromatography for intact therapertic proteins and their subunit analyses using MAbPac RP column; Xuefei Sun1; Zoltan Szabo1; Brandon H. Robson1; Shanhua Lin1; Mike Baynham2; Rainer Bauder3; 1Thermo Fisher Scientific, Sunnyvale, CA; 2Thermo Fisher Scientific, Runcorn, United Kingdom; 3Thermo Fisher Scientific, Cambridge, MA

MP 524 Intact analysis and binding site determination of covalent ibritinib adduct with human serum proteins by LC-triple TOF mass spectrometer; Ming Yao1; Jinping Gan1; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb Company, Princeton, NJ

MP 525 Automating the characterization of ambiguity in proteoform identifications with discovery top-down proteomics; Richard Leduc1; Ryan Fellers2; Bryan P Early2; Joe Greer2; Paul Thomas2; Michael R. Shortreed3; Lloyd M. Smith3; Neil L Kelleher3; 1Northwestern University, Bloomington, IN; 2Northwestern University, Evanston, IL/60208; 3University of Wisconsin-Madison, Madison, Wisconsin

MP 526 Aging in the mouse brain is associated with increased histone methylation on histone H3.3; Karl Poncha1; Tao Wang2; Matthew Holt2; Nicolas L. Young2; 1BCM, Houston; 2BCM, Houston, Texas

PROTEOMICS: NEW APPROACHES I

MP 527 Development of an Efficient Method for Biotinylated Protein Purification Coupled with Tandem Mass Tag Mass Spectrometry; Huan Sun1; Xiaojun Sun1; Junmin Peng1, 2; 1Departments of Structural Biology and Developmental Neurobiology, St. Jude Children’s Research Hospital, Memphis, TN; 2Center for Proteomics and Metabolomics, St. Jude Children’s Research Hospital, Memphis, TN

MP 528 GloboQuant-A method for Proteome-wide absolute quantification; Bharath Kumar RaghuRaman1; Ignacy Rzagaliniski1; Andrej Shevchenko1; 1Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

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Chemical probe with α-methylene-β-lactone warhead labeling diverse classes of enzymes; Lei Wang1; Louis P. Riel1; Bekim Bajrami2; Bin Deng3; Amy R. Howell1; Xudong Yao1; 1Department of Chemistry, University of Connecticut, Storrs, CT; 2Chemical Biology & Proteomics, Biogen, Cambridge, MA; 3Department of Biology, University of Vermont, Burlington, VT

Robust, reproducible and quantitative analysis of thousands of proteomes by micro-flow LC-MS/MS; Yangyang Bian1; Runsheng Zheng1; Florian P. Bayer1; Cassandra Wong2; Yun-Chen Chang3; Chen Meng3; Daniel P. Zolg1; Maria Reinecke1; Jana Zecha1; Svenja Wiechmann1; Stephanie Heinzelmeir1; Johannes Scherr1; Bernhard Hammer2; Mike Baynham6; Anne-Claude Gingras2; Oleksandr Boychenko3; Bernhard Kuster1; 1Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 2Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, Ontario; 3Bavarian Biomolecular Mass Spectrometry Center (BayBioMS), Technical University of Munich, Freising, Germany; 4Centre for Preventive and Sports Medicine, Klinikum Rechts der Isar, Technical University of Munich, Munich, Germany; 5Department of Neurology, Klinikum Rechts der Isar, Medical Faculty, Technical University of Munich, Munich, Germany; 6Thermo Fisher Scientific, Runcorn, United Kingdom; 7Thermo Fisher Scientific, Germering, Germany

Bead Assisted Mass Spectrometry (BAMS™) Enables Effectively Instantaneous Transformation of MS1 Peak Lists to Quantitative Pathway Reports; Sergey Mamaev1; Manor Askenazi2; Camilla Worsfold1; Jeffrey C. Silva1; Vladislav B. Bergo1; 1Adeptrix Corporation, Beverly, MA 01915; 2Biomedical Hosting LLC, Arlington, MA 02474

Expanding Proteome Coverage through the Use of Lysoobacter Capsici beta-lytic Metalloendopeptidase; Mikhail Konstantinov1; Alexey Afoshin2; Irina Kudryakova2; Natalia Vasilyeva2; Ilya Toropygin2; 1Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; 2G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Pushchino, Russia; 3Inst. of Biomedical Chemistry, Moscow, Russian Federation

The Julienne method improves depths of proteome coverage and LC/MS throughput; Thomas Clark1; Queenie Chen1; Nik Stoynov2; Greg Stacey1; Karina Nielsen1; Michael Skinnider1; Leonard Foster1; 1UBC, Vancouver, BC

Absolute Quantitation of Proteins by Coulometric Mass Spectrometry; Pengyi Zhao1; Qi Wang1; Manpreet Kaur1; Yong-Ick Kim1; Howard D Dewald1; Hao Chen1; 1New Jersey Institute of Technology, Newark, NJ; 2 Ohio University, Athens, OH

Heat and Beat (HnB): A one-pot rapid tissue sample preparation technique for proteomics in under an hour; Dylan Xavier1; Clare Loudon1; Peter G Hains1; Philip J Robinson1; 1Children’s Medical Research Institute, Westmead, Australia; 2University of Sydney, Camperdown, Australia

Trypsin Limited Proteolysis Strategy towards in-depth Structural Proteomics; Kosuke Ogata1; Yasushi Ishihama1; 1Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan

CtpCP in the act: Degradomics investigation of CtpCP-substrates; David Mario Ho1; 2; Julia Leodolter1; Markus Hartl2; Tim Clausen1; 1Institute of Molecular Pathology (IMP), Vienna, Austria; 2Max Perutz Labs, Vienna, Austria

Turnkey, multi-pathway signaling analysis using a synthetic phosphopeptide panel, standardized sample preparation kits and SureQuant standard target quantitation; Aaron S Gajadhar1; Bhavin Patel2; Penny Jensen2; Sebastian Gallien1; 3; 4; Romain Huguet5; Kay Opperman5; John C Rogers1; Andreas Huhmer5; Daniel Lopez-Ferrer2; 1Thermo Scientific, San Jose, CA; 2Thermo Fisher Scientific, Rockford, IL; 3Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; 4Thermo Fisher Scientific, Paris, France; 5Thermo Fisher Scientific, Bremen, Germany

Comprehensive and robust proteome profiling using Online-2D nanoLC coupled to the Orbitrap Explorist 480 MS; Tabiwan N. Arrey1; Runsheng Zheng2; Oleksandr Boychenko2; Alexander Harder2; 1Thermo Fisher Scientific, Bremen, Germany; 2Thermo Fisher Scientific, Germering, Germany; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

Robust Label-Free Proteomics Analysis with a New Orbitrap Mass Spectrometer, FAIMS Separation and micro-Pillar Array columns (uPAC) chromatography; Khaterah Motamedchakaboki1; Aaron S. Gajadhar1; Aman Makaia2; Yang Liu2; Julia Kraegenbring1; Tabiwan N. Arrey2; Geert Van Raemdonck1; Ali Perez2; David M Horn3; Alexander Harder1; Daniel Lopez-Ferrer2; 1Thermo fisher scientific; 2Thermo fisher scientific, San Jose, CA; 3Thermo Fisher Scientific, San Jose, California; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 5PharmaFluidics, Technologiepark-Zwijndaele 82, Gent, Belgium

Deep proteome coverage and label-free proteomic analysis of low numbers of mammalian cells with a quadrupole-ion-trap-Orbitrap mass spectrometer; Min Huang1; Xiuxiu Sun1; Yue Zhou1; 1Thermo Fisher Scientific, Shanghai, China
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MP 543  Single cell HbA1C measurement using isotope dilution mass spectrometry to determine erythrocyte age; Azad Esghii1; Darryl Hardie1; Ying Zhu2; Ryan T Kelly2,3; David R Goodlett1,5; 1uvic genome bc protein centre, victoria; 2Pacific Northwest National Lab, Richland, WA; 3Bingham Young University, Provo, UT; 4University of Maryland, Baltimore, Baltimore, MD; 5University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland

MP 544  Single Cell Proteomics and the Carrier Proteome Effect; Bernhard Kuster1; Christopher M. Rose2; 1Proteomics and Bioanalytics, Technical University of Munich, Germany; 2Discovery Proteomics, Genentech Inc., So. San Francisco, CA

MP 545  Cell Classification Using Single Cell Mass Spectrometry Through Interpretable Machine Learning; Yuxuan Xie1; Daniel C Castro1; Sara E Bell1; Stanislav Rubakhin1; Jonathan V Sweedler1; 1University 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 Choi1; Peter Nemes1; Abigail Poller2; 1University of Maryland College Park, College Park, MD; 2George Washington University, Washington, DC

MP 547  PASEF for sensitive shotgun proteomics: toward single cell analysis; Thomas Kosinski1; Ning Chen2; Markus Lubeck1; Heiner Koch1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker (Beijing) Scientific Technology Co., Ltd., Beijing, China

MP 548  High Sensitivity Top-Down Proteomics of Single Muscle Fibers; Jake A. Melby1; Yutong Jin2; Kyle Brown2; Yanlong Zhu2; Ziqing Lin3; Gary Differe2; Ying Ge4; 1University of Wisconsin-Madison, Madison, WI; 2University of Wisconsin-Madison-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 Mizuno1; Natsumi Tanaka1; Takamitsu Sasaki1; Iwao Sakane2; Eiji Sugiyama1; Toshimasa Toyo’oka1; Kouichi Yoshinari1; Shinobu Kudoh3; Kenichiro Todoroki1; University of Shizuoka, Shizuoka, Japan; 1TO-EN LTD, Tokyo, Japan; 2Yokogawa Electric Corporation, Musashino, Japan

MP 550  Improved single-cell proteome coverage by integration of nanoPOTS and SMTA chemical labeling mass spectrometry; Santosh A. Misal1; Amanda J. Guise2; Yongzheng Cong1; Edward D. Plowey1; Samuel Payne1; Ryan T. Kelly1; 1Brigham Young University, Provo, UT; 2Biogen, Inc., Cambridge, Massachusetts

MP 551  Toward Low-Input Metabolomics using Microfluidic Sample Preparation; Steven R Doonan1; Gary Patti1; 1Washington 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 Williams1; Andrey Liu1; Chia-Feng Tsai1; Ronald J. Moore1; Daniel J. Orton1; William B. Chrisler1; Gaffrey J. Mathew1; Tao Liu1; Ryan T. Kelly2; Richard D. Smith1; Lilijana Pasa-Tolic1; Ying Zhu1; 1Pacific Northwest National Laboratory, Richland, WA; 2Bingham Young University, Provo, UT

MP 553  Single-cell proteome analysis combining nanoPOTS, nanoLC and FAIMSpro increases coverage to >1000 proteins/cell; Yongzheng Cong1; Khaterer Motamedchaboki2; Santosh A. Misal1; Yiran Liang1; Amanda J. Guise2; Thy Truong1; Yufeng Shen1; Romain Huguet2; Daniel Lopez-Ferrer3; Edward D. Plowey2; Ying Zhu2; Ryan T. Kelly1,5; 1Brigham Young University, Provo, UT; 2Thermo Fisher Scientific, San Jose, CA; 3Biogen, Inc., Cambridge, Massachusetts; 4CoAnn Technologies, LLC, Richland, Washington; 5Pacific Northwest National Laboratory, Richland, WA

MP 554  Comprehensive Single Cell and Bulk Proteomic Analyses of Human Cellular Models for HIV Reactivation; Soham Gupta1; Jimmy E Rodriguez1; Ujjwal Neogi1; Roman A Zubarev1; Akos Vegvari1; 1Karolinska Institutet, Stockholm, Sweden

MP 555  Single-Cell Deep Lipidomics via Photochemical Reaction and Tandem Mass Spectrometry; Zishuai Li1; Simin Cheng1; Qiaohong Lin1; Wenbo Cao1; Jing Yang1; Wenpeng Zhang1; Yu Xia1; Zheng Ouyang1; Xiaoxiao Ma1; 1Tsinghua 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 Cortecka1,2; Gabriela Krňšáková1; Florian Stanek1; Karel Stejskal2; Josef M. Penninger1,2; Karl Mechtler1,2; Johannes Stadlmann2; 1IMP, Vienna, Austria; 2Institute of Molecular Biotechnology, Austrian Academy of Sciences (IMBA), Vienna, Austria; 3Department 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 Specht1; Edward Emmott1; Aleksandra Petelski1; R. Gray Huffman1; Hendrik Wesseling2; Marco Serra3; Peter Kharchenko3; Erik Hett8; David H Perlman8; Antonius Koller8; Nikolai Slavov8; 1Department of Bioengineering and Barnett
**INSTITUTE, Northeastern University, Boston, MA; 2Merck Exploratory Sciences Center, Merck & Sharp & Dohme Corp, Cambridge, MA; 3Department 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 Zhu1; Wenhua Wang1; Zhibo Yang1; 1University 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 Chen1; Zhibo Yang1; 1University 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 Kraegenbring1; Karel Stejskal2; Otto Hudec2; Gabriela Krssakova2; Jeff Op De Beeck3; Tabeiang N. Arrey4; Bernard Delanghe4; Alexander Harder4; Kari Mechtler2, 5; 1Thermo Fisher Scientific, Bremen, Germany; 2Institute of Molecular Biotechnology, Austrian Academy of Sciences (IMBA), Vienna, Austria; 3PharmaFluidics, Technologiekpark-Zwijnarde 82, Gent, Belgium; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 5IMP, Vienna, Austria

**MP 561** Exploratory approaches to highly-sensitive analysis toward single-cell shotgun proteomics using nano-LC/MS/MS; Kosuke Hata1; Takeshi Hara1; Yoshihiro Izumi1; Masaki Matsumoto1, 2; Takeshi Bamba1; 1Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; 2Department 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 Zhang1; Norman Dovichi1; 1University of Notre Dame, Notre Dame, IN

**MP 563** Comparative MALDI MS analysis of human pancreatic islets – from tissues to individual cells; Stanislav Rubakhin1; Jonathan V Sweedler1; 1Beckman Institute, UIUC, Urbana, IL; 2Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL

**MP 564** High Precision UV Ablation Sampling for MALDI Mass Spectrometry; Kelcey B Hines1; Fabrizio Donnarumma2; Kermit K. Murray3; 1Louisiana State University, Baton Rouge, LA; 2Louisiana 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 Scheibal1; Michal Gregus1; James Kostas1; Joanna Lee1; Alexander R. Ivanov1; 1Barnett 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 Motamedchaboki1; Maowei Dou1; Yongzheng Cong1; Romain Huguet2; Aaron M Robitaille3; Yufeng Shen4, 7; Daniel Lopez-Ferrer5; Ryan T. Kelly5; Ying Zhu6; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Rockford, IL; 3Brigham Young University, Provo, UT; 4Thermo Fisher Scientific, San Jose, California; 5Thermo Fisher Scientific, San Jose, CA; 6CoAnn Technologies LLC, Richland, WA; 7CoAnn Technologies, LLC, Richland, Washington; 8ThermoFisher Scientific, San Jose, CA; 9Pacific Northwest National Laboratory, Richland, WA

**MP 567** Single Cell-ICP-MS, an Emerging Technology to Study Microorganisms; Honglan Shi; Missouri University of Science 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 Nakatani1; Yoshihiro Izumi1; Kosuke Hata1; Takeshi Bamba1; 1Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan

**TOXICOLOGY**

**MP 569** Multiplex Quantitation of Biomolecules Involved in Copper Toxicity via Custom N,N-Dimethylated Leucine (DiLeu) 12-plex Isobaric Tags; Christopher S Sauer1; Mason A Job1; Lingjun Li1; 1University 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 Macmillan1; Mihaela Mocanu1; Joseph Strasser2; Vicki M. Richardson1; 1USEPA/ORD/CCTE, Durham, NC; 2Oak 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 Schrunk1; Laura E Burns1; Scott Peterman2; Caroline Ding2; Brandon Bills3; Ed George2; Kizito Nishimwe4; Graeme Mcalister2; Seema Sharma5; Iowa State University, Ames, IA; 2Thermo 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 Tansrisawad1; Udomsak Hoonwijit1; Apinya

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<td>Department of Forensic Medicine, Chulalongkorn University, Bangkok, Thailand; Department of Forensic Medicine, King Chulalongkorn Memorial Hospital, The Thai Red Cross Society, Bangkok, Thailand; Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; Bara Scientific Co., Ltd., Bangkok, Thailand</td>
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<td>Jonathan Rochon; Jean Lacoursière; Serge Auger; Francis Brière; Pier-Luc Plante; Pierre Picard</td>
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<td>Department of Forensic Medicine, Chulalongkorn University, Bangkok, Thailand; Department of Forensic Medicine, King Chulalongkorn Memorial Hospital, The Thai Red Cross Society, Bangkok, Thailand; Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; Bara Scientific Co., Ltd., Bangkok, Thailand</td>
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<td>MP 578 Controlling Crosstalk of Amphetamine and Methamphetamine in Urine Assays Using 96 well plates for LC-MS/MS Analysis</td>
<td>Stephanie Marin; Mario Merida; Jeremy Smith; Elena Gairloch</td>
<td>Biotage, Charlotte, NC</td>
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<td>MP 579 Rapid Detection of Growth Hormone-Releasing Peptides in Dried Blood Spots</td>
<td>Pierre Negri; Enrico Gerace; Jessica Modaffari; Daniele Dicorcia; Marco Vicenti; Alberto Salomone</td>
<td>Centro Regionale Antidoping e di Tossicologia “A. Bertinaria”, Turin, Italy; Dipartimento di Chimica, Universita' degli Studi di Torino, Torino, Italy</td>
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<td>MP 580 Detection of Fentanyl Analogs and Novel Synthetic Opioids in Hair</td>
<td>Pierre Negri; Daniele Dicorcia; Alberto Salomone</td>
<td>SCIEX, Redwood City, CA; Centro Regionale Antidoping e di Tossicologia “A. Bertinaria”, Turin, Italy</td>
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<td>MP 581 Rapid Detection of Isomeric Fentanyl Analogs at Trace Levels using LC-TIMS-TOF MS</td>
<td>Elisa N Shoff; Cesar E. Ramirez; Francisco A. Fernandez-Lima</td>
<td>Miami-Dade Medical Examiner Department, Miami, FL; Florida International University, Miami, FL</td>
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**MONDAY POSTERS (MP) Pages 5-44 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.**
Identification of Tryptophan Metabolites in Brain Tissue Using Paper Spray Ionization-Mass Spectrometry; Marco V Melgar1; Richard C Dilworth1; Vanessa Y Rubio1; Gary P Wang1; Timothy J Garrett1; 1University of Florida, Gainesville, FL

Ultrasonic Nebulizer Assisted Atmospheric-Pressure Chemical Ionization (APCI) for Explosives analysis; Linxia Song1; Theresa Evans-Nguyen1; 1University of South Florida, Tampa, FL

Ultrafast qualitative screening of mitragynine, MDMA, and tetrahydrocannabinol (THC) in complex matrices by green technology direct probe ionization mass spectrometry; Udi Jumhawan1; Saravana Kumar Jayaram2; May Yen Ang3; Hazni Hashim3; Muhammad Hafiz Zulkiflee2; Nur Nazihah Md Shahari2; Wan Rahimah Wan Ahmad2; Sandhya Aniruddha Nargund1; Lai Chin Hui-Loo1; 1Shimadzu Asia Pacific, Singapore, Singapore; 2Division of Narcotics, Department of Chemistry Malaysia, Petaling Jaya, Malaysia; 3Shimadzu Malaysia, Petaling Jaya, Malaysia

Thermal Desorption Enabled Electrospray and DART Ionization of Solids and Inorganic Salts; Frederick Li1; Paul Liang1; Scott Oro1; Brittany Laramee1; Kenyon Evans-Nguyen2; Brian Musselman1; 1IonSense, Inc., Saugus, MA; 2University of Tampa, Tampa, FL

Skip Sample Preparation and Facilitate Analysis of Food by Screening via the 24-Pin Sampler with DART-MS; Brittany Laramee1; Frederick Li1; Paul Liang1; Brian Musselman1; 1IonSense, Inc, Saugus, MA

Real-Time Monitoring of Cellular Metabolism by Dual-Probe Microsampling Integrated with Multiplexed Ion Mobility-Mass Spectrometry; Taylor M Domenick1; Richard A Yost1; Vinata Vedam-Mai1; 1University of Florida, Gainesville, FL

Microdroplet-accelerated Synthesis of Substituted Benzimidazoles; Pallab Basuri1, 2; L. Edwin Gonzalez1; Thalapip Pradeep2; R. Graham Cooks1; 1Purdue University, West Lafayette, IN; 2Indian Institute of Technology, Madras, Chennai, India

Mass spectrometry analysis reveals metabolic discrepancies between histologically equivalent tissues that may hamper utility in molecular models; Michael Woolman1; Lauren Katz1; Georgia Gopinath1; Taiara Kiyota1; Claudia Kuzan-Fischer1; Isabelle Ferry1; Megan Wu1; Sunit Das1; Michael D Taylor1; James Rutka1; Howard Ginsberg1; Ahmed Aman1; Arash Zarrine-Afsar1; 1University of Toronto, Toronto, ON; 2Ontario Institute for Cancer Research, Toronto, ON

Post-acquisition Data Analysis Program for Automating Data Processing in High-throughput Experimentation with DART-MS; Robert Goguen1; Frederick Li1; Paul Liang1; Brittany Laramee1; Brian Musselman1; 1IonSense, Inc, Saugus, MA

Diagnosis of metabolic diseases by discriminative biofluid fingerprinting: reaching the next level with laser-assisted rapid evaporative ionization mass spectrometry (LA-REIMS); Lieven Van Meulebroek1; Ellen De Paepe1; Kathleen Wijnam1, 2; Vera Plekhoava1; Margot De Spiegeleer1; Bruno Lapauw1; Nathalie Michels1; Stefaan De Henauw1; Myriam Van Wincfel1; Lynn Vanhaecke1, 5; 1Ghent 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

In situ tissue pathology from spatially encoded mass spectrometry classifiers visualized in real time through augmented reality; Michael Woolman1; Jimmy Qiu2; Claudia Kuzan-Fischer1; Isabelle Ferry1; Delaram Dara1; Lauren Katz1; Fowad Daud1; Megan Wu1; Manuela Ventura1; Nicholas Bernards2; Harley Chan1; Inga Fricke1; Mark Zaidi1; Michael D Taylor1; James Rutka1; Jonathan Irish1; Robert Weersink2; Howard Ginsberg1; David Jaffray1; Arash Zarrine-Afsar1; 1University of Toronto, Toronto, ON; 2University Health Network, Toronto, ON; 3Thermo Fisher Scientific, San Jose, CA; 4ThermoFisher Scientific, San Jose, CA

High-throughput assay and intact protein analysis by liquid AP-MALDI MS; Henriette Krenkel1; Evita Hartmane1; Cristian Piras1; Jeffery Brown1, 2; Michael Morris2; Rainer Cramer1; 1University of Reading, Reading, United Kingdom; 2Waters Corporation, Wilmslow, United Kingdom

Application of VeriSpray ion source Triple Quadrupole Mass Spectrometry for the analysis of stimulants and narcotics in oral fluid; Gustavo de Albuquerque Cavalcanti1; Yu Zhu2; Wijeratne Neloni2; Claudia Martins3; 1Brazilian Doping Control, Rio de Janeiro, Brazil; 2Thermo Fisher Scientific, San Jose, CA; 3ThermoFisher Scientific, San Jose, CA

Rapid Screening of High Priority N-Nitrosamines in Pharmaceutical, Forensic, and Environmental Samples with FCSI-MS and PSI-MS; Trevor J. McDaniel1; Jessica M. Holtz1; Makoy Overfelt1; Christopher C. Mulligan1; 1Illinois 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; Brian D. Musselman1; Paul Liang2; Scott Oro; Brittany Laramee3; Frederick Li4; IonSense, Inc., Saugus, MA; 1IonSense, 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; Eshwar Jagerdeo1; Serge Auger2; FBI, Springfield, VA; 2Phytronix Technologies, Inc., Quebec, QC

TP 018 Rapid Detection of 25 Types of Drugs by DART Coupled with Ultivo Triple Quadrupole MS; Jianzhong Li1; Kerry Song2; Xiaokun Duan3; Agilent Technologies, Beijing, China; 2ASPEC Technologies, Beijing, China

TP 019 Identification of Random or Block Copolymers by Pyrolysis DART-MS: A Comparison Study with Pyrolysis GC-MS; Ruilin Hu1; Dongyan Mao1; Xiaokun Duan2; Kerry Song2; Charles C. Liu2; BASF Advanced Chemicals Co., Ltd., Shanghai, China; 2ASPEC Technologies, Beijing, China

TP 020 Pulse DART: Improving Throughput and Reducing Helium Consumption, Ambient Background and Matrix Interference; Scott Oro3; Frederick Li4; Paul Liang2; Brittany Laramee3; Brian Musselman1; IonSense, Saugus, MA; 1IonSense, Inc. Saugus, MA

TP 021 Reproducibility of native SEC LC-MS intact mAb characterisation measurements; Dirk Wunderlich1; Christian Albers1; Sylvia Jozwiak; Karina Bora; Ben Wilkses2; Bruker Daltonik GmbH, Bremen, Germany; 2Lonza, Slough, United Kingdom

TP 022 The HOS and thermal stability of six biotherapeutic antibodies based on mobility measurements of singly-charged electrospray ions at atmospheric pressure; Henry Benner1; Ben Aguilar1; Ion Dx, Monterey, CA

TP 023 Profiling in vivo and in vitro Biotransformation of Biotherapeutics by Immunoaffinity LC-MS/MS; Suk-Joon Hyung1; Surinder Kaur1; Ola Saad1; Genentech, South San Francisco, CA

TP 024 Development of a New Workflow for Multiple Attribute Monitoring (MAM) of an Antibody-Drug-Conjugate (ADC); Armelle Martelet1; Valérie Garrigue1; Hélène Le Borgne1; Bruno Genet1; Zoe Zhang1; Kerstin Pohl3; SANOFI, Vitry sur seine, France; 2SciEX, Redwood Shores, CA; 3SciEX, Framingham, MA

TP 025 Implementing MHC Associated Proteome Imaging (MAPPs) in drug development and immunogenicity risk assessment; Jason Lamar1; Sylvia Wong1; Violet Lee2; Lynn Kamen2; Azadeh Hassanzadeh2; Han Chung3; Surinder Kaur1; Ola Saad1; Genentech - South San Francisco, CA, SSF, CA; 2Genentech, South San Francisco, CA

TP 026 Automated affinity capture LC-MS methods for bioanalysis of Antibody Drug Conjugates (ADCs) and antibody fusion proteins; Madhura Deshpande1; Srikanth Kotapati1; Aarti Jashnani1; Jason Hogan1; Gavin Dollinger1; Arvind Rajpal1; Bristol-Myers Squibb, Redwood City, CA

TP 027 High resolution LC/MS characterization of site-specific antibody-drug conjugate synthesized by CCAP method; Kenji Hirose1; Taiji Kawase1; Satoshi Kishimoto2; Takaaki Hatanaka3; Motoyasu Adachi3; Yuji Ito2; Nihon Waters K.K., Osaka, Japan; 2Kagoshima University, Kagoshima, Japan; 3National 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 Immunoaffinity LC-MS/MS; Kristin Geddes1; Yaping Liu2; Eberhard Durr2; Arthur Friedman2; Zhifeng Chen2; Toya Nath Baral3; Daniel S Spellman2; Merck & Co., Inc., West Point, PA; 2Merck and Co, Inc, West Point, PA; 3Merck & Co., Inc., South San Francisco, CA

TP 029 Reproducibility of native SEC LC-MS intact mAb characterisation measurements; Dirk Wunderlich1; Christian Albers1; Sylvia Jozwiak; Karina Bora; Ben Wilkses; Bruker Daltonik GmbH, Bremen, Germany; Lonza, Slough, United Kingdom

TP 030 Enhancing Host-Cell Protein Detection in Protein Therapeutics Using HILIC Enrichment and Proteomic Analysis; Qingyi Wang1; Thomas R. Slaney1; Wei Wu1; Richard Ludwig1; Li Tao1; Anthony Leone1; Bristol-Myers Squibb Company, Pennington, NJ

TP 031 Interlaboratory study of an optimized peptide mapping workflow using automated trypsin digestion for monitoring product quality attr; Silvia Millan Martin1; Craig Jakes1,2; Sara Carillo1; Tom Buchanan3; Marc Guender4; Dan Bach Kristensen5; Ken Cook6; Jonathan Bones7; NIBRT, Dublin, Ireland; 2School of Chemical Engineering and Bioprocessing, University College of Dublin, Dublin, Ireland; 3Thermo Fisher Scientific, Hemel, United Kingdom; 4Thermo Fisher Scientific, reinach, Switzerland; 5Symphogen, Ballerup, Denmark

TP 032 A Comprehensive Assessment of Chemical Liabilities in 84 Different SEFL2 IgG1 mAbs; Chen-Chun Chen1; Andrew B. Dykstra1; Alex W. Jacobitz1; Neelam Khanal1; Chris Spahr1; Kenneth Walker1; Daniel Yoo1; Wei Zhang2; Yang Yuan Sheng2; Nic Angell1; Iain D. G. Campuzano1; Amgen Inc., Thousand Oaks, CA; 2Agency for Science, Technology and Research, Singapore, Singapore

TP 033 A labeling strategy to improve peptide fragmentation and to distinguish isobaric amino acids by EThcD; Thierry Le Bihan1; Jin Duan2; Zac McCandall2; Xin Xu2; Paul Taylor2; Qixin Liu2; Kathleen Gorseps1; Bin Ma1,2; Rapid Novor Inc, Kitchener; 2University 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; Xiaoli Zhang1; Hao Yang2; Haichuan Liu2; Min Du3; 1ThermoFisher Scientific, Shanghai, China; 2ThermoFisher Scientific, San Jose, California; 3ThermoFisher Scientific, Massachusetts, Massachusetts |
| **TP 035** | Site-Specific Conjugation Analysis of an Antibody Drug Conjugate Mimic by Peptide Mapping; Ken Chanthamontri1; Benjamin Cutak1; Kevin Ray1; MilliporeSigma, St. Louis, MO |

### BIOMARKERS: DISCOVERY I

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| TP 037 | Examining effects of increased cytosolic acetyl-CoA levels on Ne-lysine acetylation through proteomic analysis of SLC13A5 and SLC25A1 overexpression; Hannah Miles1; Min Ma1; Michael J. Rigby2; Nicola Salvatore Orfice3; Luigi Puglielli3; Lingjun Li1, 3; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; 2Department of Medicine and Waisman Center, University of Wisconsin-Madison, Madison, WI 53705; 3Department 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 Gauthier1; Gréogy Leclerc1; Aude Le Gall1; Jérôme Dupuis1; Brian Lockhart1; Emmanuel Nony1; 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 Govender1; Demetra Mavri-Damelini1; Previn Naicker1; Faheem Seedat1; Neil Martinson2, 3;1Ebrahim Varia2;1Dalu Mancama;1Stoyan Stoychev1; 2Council for Scientific and Industrial Research, Pretoria, South Africa; 3University of the Witwatersrand, Johannesburg, South Africa; 4Johns Hopkins University School of Medicine, Baltimore, Maryland |
| TP 042 | Advanced Biomarker Discovery in Imaging Mass Spectrometry Through Interpretable Supervised Machine Learning; Leonoor Ella Marie Tideeman1; Lukasz G. Migas1; Emilio Rivera2, 3; Katerina V. Djambazova2, 4; Elizabeth Neumann2, 3; Nathan Heath Patterson2, 3; Richard M Caprioli2, 3; Jeffrey M Spraggins2, 3; Raf Van De Plas1, 2, 3; 1Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; 2Mass Spectrometry Research Center, Nashville, TN; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Chemistry, Vanderbilt University, Nashville, TN; 5Department of Medicine, Vanderbilt University, Nashville, TN; 6Department of Pharmacology, Vanderbilt University, Nashville, TN |
| TP 043 | Investigation on Coagulation Responsive Proteins in Human Serum using Proteomic Techniques; Abu Hena Mostafa Kamal1; Kevin Zhu2; Madison Roberts2; Gul Nowshad1; Lina Ab Mosleh1; Mohamad Ammar Ayass1; 1Ayass BioScience, LLC, Frisco, TX; 2University of Wisconsin-Madison, Madison, WI |
| TP 044 | Identification and characterization of extracellular matrix proteins enabled by a photo-cleavable surfactant; Samantha J Knott1; Kyle Brown1; Harini Josyer2; Stanford Mitchell3; Austin Carr2; David Inman4; Suzanne Ponik4; Andreas Friedl5; Ying Ge1, 4, 6; 1Department of chemistry, University of Wisconsin Madison, Madison, WI; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 3Department of Molecular and Cellular Pharmacology, University of Wisconsin-Madison, Madison, WI; 4Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI; 5Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; 6Director 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 Whitham1; Roshanak Aslebagh2; Devika Channaveerappa3; Brian Pentecost3; Kathleen F. Arcaro2; Costel C. Darie1; 1Clarkson University, Potsdam, NY; 2University of Massachusetts Amherst, Amherst, MA |
| TP 046 | Identification and quantification of cholangiocarcinoma (CCA) marker proteins from bile extracellular vesicles for non-invasive diagnosis; Ayako Kurimoto1; Tatsutoshi Inuzuka1; Toshiki Ueda1; Chisaki Ikeda2; Hiroaki Haga2; 1Miraca Research Institute G.K., Tokyo, Japan; 2Department 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 Kuruc1; Swapan Roy1; Wilma Mesker1; Rob Tollenaar1; 1Biotech Support Group LLC, Monmouth Junction, NJ; 2Leiden University Medical Center, Leiden, Netherlands |
TP 049  Targeted proteomics of cerebrospinal fluid biomarkers in Alzheimer’s disease; Maotian Zhou1; Rafi U Haque1; Eric B. Dammer2; Duc M. Duong3; Lingyan Ping1; Erik C.B. Johnson2; James J. Lah2; Allan Levey2; Nicholas T Seyfried2; 1Emory University, atlanta, GA; 2Emory University, Atlanta, GA

TP 050  Identification of Salivary Proteins Responsible for a Peptide Fragment to be used as a Diagnostic Test for sjøgren Syndrome; Abhijit Roychowdhury1; Jasmin De Luna1,2; Earl L White3; 1MDx BioAnalytical Laboratory, Inc., College Station, TX; 2Blinn College, Bryan, Texas; 3MDx BioAnalytical Laboratory, Inc., College Station, Texas

TP 051  Pilot Study of Untargeted Urine Metabolomics in Sarcoma Patients Treated with HD-AIM; Garrett Kinnebrew1; Joseph Mcelroy1; David Liebner2; James L Chen3; Ewy Mathe1; 1The 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 Kim1; Jun Hyung Lee1; Sunghyun Huh1; Seo Young Sim2; Jinnyoung Choi3; Seung Hyeun Lee2,4; 1DGIST, Daegu, South Korea; 2Kyung Hee University, Yongin, South Korea; 3Bruker Daltonics Korea, Seoul, South Korea; 4Kyung 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 Imran1; Paulos Chumala1; Mary Buhr1; George S. Katselis1; 1University 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 Jain1; Alexander B. Saltzman1; Jong Min Choi1; Ruya Liu2; Barbara M Brooks-Worrell3; Jerry P Palmer4; Vijay K Yechoor5; Sung Yun Jun1; Erica G Hattery5; Ashok Balasubramanyam5; Anna Malovannaya5; 1Bay College of Medicine, Houston, TX; 2University of Pittsburgh, Pittsburgh, PA; 3University of Washington, Seattle, WA; 4DVA Puget Sound Health Care System, Seattle, WA

TP 056  Quantitative biomarker to assess teratogenicity of DHODH inhibitors in vivo; Michael A Pontikos1; Christopher Leija1; Xiaoyu Wang1; Noelle S Williams1; Margaret A Phillips3; 1University of Texas Southwestern Medical Center, Dallas, TX

TP 057  Proteomic Biomarkers of Multimparametric Magnetic Resonance Imaging Visibility in Prostate Cancer; Amanda Khoo1; Taylor Y. Sadun2; Vladimir Ignatchenko3; Lydia Y. Liu1; Aydin Pooli2; Katie Houlanan1; Steven S. Raman1; Anthony E. Sisk Jr.1; Paul C. Boutros4; Robert E. Reiter1; Thomas Kislinger1,3; 1University of Toronto, Toronto, ON; 2Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA; 3Princess 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 Zheng1; Kristin Taylor1; Rong Liu1; Scott Robotham1; Rasa Santockyte1; Lihong Cheng1; Yi Luo1; Yan J. Zhang1; Renuka Pillutla1; Jianing Zeng1; 1Bristol-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 Zhang1; Charles River Laboratories, Worcester, MA

TP 060  A Methyalted Protein Biomarker of Target Engagement in Blood and Tumors: From Proteomic Screen to Clinical Assay; Timothy Sikorski1; Paul Noto1; Francesca Zappacosta2; Craig Wagner1; Rocio Montes De Oca1; Matthew Szapacs1; Roland S Annan1; 1University Health Center, Montreal, QC; 2Blinn College, Bryan, Texas; 3MDx BioAnalytical Laboratory, Inc., College Station, Texas

TP 061  A Multiomic Evaluation the Effects of Exercise and Menopause on Cognition in Alzheimer’s Disease Mouse Models; Kendra J. Adams1; Janai Williams1; Lisa St. John-Williams1; Sarah Hiles1; Carol A. Colton1; M. Arthur Moseley1; Christina L. Williams1; 1Duke University, Durham, NC

TP 062  A Sensitive Immuno-MRM Assay for Quantifying PTEN to Allow Better Stratification of Breast Cancer Patients; Sahar Ibrahim1; Naciba Benlimame2; Adriana Aguilar-Mahecha3; Alan Spatz4; Mark Basik5, 6; Gerald Batist5, 6; Constance A. Sobsey1; Christoph H. Borchers1, 5, 6; René Zahedi1; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Pathology Research Department, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 3Cancer Genomics and Translational Research Laboratory, Segal Cancer Center, Lady Davis Institute for Medical Research, Sir Mortimer B. Davis Jewish General Hospital, Montreal, QC; 4Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; 5Segal Cancer Center, Lady Davis Institute for Medical Research, Sir Mortimer B. Davis Jewish General Hospital, McGill University, Montreal, QC; 6Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 7Department 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 Li1; Bang-lin Wan1; Guangping Bi1; Rena Zhang1; Daniel S Spellman1; 1Merck & 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); Ji hyeon Lee1; Areum Sohn1; Sangjin Rhee2; Yongmin Ahn2; Youngsoo Kim1, 3; 1Department of Biomedical Sciences, Seoul National University, Seoul, South Korea; 2Department of Neuropsychiatry, Seoul National University Hospital, Seoul, South Korea; 3Interdisciplinary 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. Murray1; Chao Dong1; Fabrizio Donnarumma1; Vincent A Ricigliano1; Touradj Solouki3; Luke Richardson1; 1Louisiana State University, Baton Rouge, LA; 2USDA-ARS Honey Bee Breeding, Genetics, and Physiology Laboratory, Baton Rouge, LA; 3Baylor University, Waco, TX

TP 067  Efficient tandem mass spectrometry method for the analysis of methylmalonic acid in urine; Tristan Martineau1; Michel Boutin1; Audrey Perreault2; Pierrette Gaudreau3; Nancy Presse1; Christiane Auray-Blais1; 1Université de Sherbrooke, Sherbrooke, QC; 2CIUSSS-de-l’Estrie-CHUS, Sherbrooke, QC; 3Université de Montréal, Montréal, QC

TP 068  A Quantitative study of potential blood biomarker for Alzheimer’s Disease by Targeted Mass Spectrometry; Yeongshin Kim1; Jaeyeon Kim1; Jooho Park1; Minsoo Son1; Youngsoo Kim1, 2, 3; 1Interdisciplinary Program of Bioengineering, Seoul National University College of Engineering, Seoul, South Korea; 2Department of Biomedical Sciences, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea; 3Department 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 Parmar1, 2; Nivedita Bhattacharya1, 2; Shanthini Kannan3; Sangetha Vadivel4; Prabhakar Sripadi4; Gokulakrishnan Kuppan3; Venkateswarlu Panchagunala4, 5; 1CSIR-National Chemical Laboratory, Pune, India, Pune, India; 2Academy of Scientific and Innovative Research (AcSIR), Pune, India; 3Madras Diabetes Research Foundation, Chennai, India; 4CSIR-Indian Institute of Chemical Technology, Hyderabad, India; 5National Chemical Laboratory, Pune, India, Pune, India

TP 070  A Standardized Workflow for Developing Protein Immunoprecipitation Assays to Support Clinical Endpoints; Brendan Tierney1; Ying Zhang1; Kyle Wald1; Matthew Blatnik1; 1Pfizer 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 Mazur1; Bogdan Slezka2; Peta Shipkova1; Timothy Olah1; 1Bristol-Myers Squibb Company, Princeton, NJ

TP 072  Serum glycoprotein markers in non-alcoholic steatohepatitis (NASH) and hepatocellular carcinoma (HCC); Prasanna Ramachandran1; Gege Xu1; Ling Shen1; Daniel Siren1; 1Intervenn 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 Ray1; Pegah Jalili1; Judy Cao1; Uma Sreenivasan1; 1MilliporeSigma, St. Louis, MO; 2MilliporeSigma, 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 Donoho1; Mona Goli1; Byeong Gwan Cho1; Alireza Banazadeh1; Firas Kobaissyp; Ryan Morgan1; Jingfu Zhao1; Endre Czeiter3, 4, 5; Krisztina Amrein3, 4, 5; Andras Buki3, 4, 5; Sakshi Gautamb; Wenjing Peng1; Stefania Mondello6, 7; Yehia Mechref8; 1Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas; 2Department of Psychiatry and Neuroscience, McKnight Brain Institute, University of Florida, Gainesville, Florida; 3Department of Neurosurgery, University of Pecs, Pecs, Hungary; 4Janos Szentagothai Research Centre, University of Pecs, Pecs, Hungary; 5MTA-PT Clinical Neuroscience MR Research Group, Pecs, Hungary; 6Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; 7Oasi Research Institute-IRCCS, Troina, Italy; 8Center 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 Simon1; Ayseguel Aksan2; Florian Bonn1; Anne Arnold1; Juergen Stein2; Franz Paul Armbrester1; 1Immundiagnostik AG, Bensheim, Germany; 2Interdisciplinary Crohn Colitis Center Rhein-Main, Frankfurt, Rhein-Main, Germany
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TP 076  Fluorinated Acyl-transfer Reagent Efficaciously Benzoylates Nucleophilic Residues for Application in Covalent-labeling Mass Spectrometry: A New Validation Workflow; Austin B. Moyle1; Ming Cheng1; Nicole D. Wagner1; Michael L. Gross1; 1Washington 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 Gracieux1; Bea Sewell1; Michael B. Goshe2; 1North Carolina State University, Raleigh, NC

TP 078  Diethylpyrocarbonate Modified Histidine Isomers Reveal Higher Resolution Protein Structural Information; Xiao Pan1; Tianying Liu2; Patanachai Kong Limpikirati2; Richard W Vachet2; 1University of Massachusetts-Amherst, Amherst, MA; 2University of Kansas Medical Center, Kansas City, KS

TP 081  Spheroid-FPOP, an Extension of In-Cell Fast Photochemical Oxidation of Proteins (IC-FPOP); Raquel Shortt1; Yijia Wang2; Amanda B. Hummon1; Lisa Jones1; 1University of Maryland Baltimore, Baltimore, MD; 2Department of Chemistry and Biochemistry, Ohio State University, Columbus, Ohio

TP 082  Crosslinked peptide support in Skyline; Nicholas Shulman1; Alex Zelter1; Michael J MacCoss1; Brendan Maclean1; 1Department of Genome Sciences, University of Washington, Seattle, WA

TP 083  Combined UV Laser Ablation and Photochemical Oxidation of Proteins for Mass Spectrometry; Oluwatosin A Ogunlade1; Fabrizio Donnarumma1; Kermit K Murray1; 1Louisiana 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. Cabrera1; Terrence G. Oas2; Michael C. Fitzgerald1; 1Department of Chemistry, Duke University, Durham, NC; 2Department of Biochemistry, Duke University Medical Center, Durham, NC

TP 085  Simple Cross-Linking/Mass Spectrometry Workflows for Studying System-Wide Protein Interactions; Claudio Iacobucci1; Michael Goetz1; Christian H Ihling1; Andrea Sinz1; 1Martin Luther University Halle, Halle, Germany

TP 086  MALDI Analysis for Protein Footprinting; Jerry Jiang1; Michael L. Gross2; 1Washington University at St. Louis, St. Louis, MO; 2Washington University in St. Louis, St. Louis, Missouri

TP 087  Can Overlabeling with DEPC Give Correct Protein Structural Information?; Zachary J Kirsch1; Richard W Vachet1; 1University 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 Zhao1; Colin P. Reilly1; James P. Reilly1; 1Indiana University, Bloomington, IN

TP 089  OpenPepXL: An open-source tool for sensitive identification of cross-linked peptides in XL-MS; Eugen Netz1; Tiegerd MH Dijkstra2; Timo Sachsenberg1; Oliver Kohlbacher1, 3, 4, 5; 1Max Planck Institute for Developmental Biology, Tübingen, Germany; 2Max Planck Institute for Developmental Biology, Tübingen, Germany; 3Applied Bioinformatics, Tübingen, Germany; 4Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; 5Institute 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 Hao1; Ying Zhang2; Zhihui Wen2; Charles A.S. Banks2; Michael P. Washburn2; 2Washington University, St. Louis, MO; 3Stowers Institute for Medical Research, Kansas City, KS

TP 091  MS-Scout: An all-rounded environment for regular and cleavable cross-linking mass spectrometry; Milan Avila Clasen1; Diogo Borges Lima2; Louise Ulrich Kurt3; Marlon Dias Mariano Dos Santos3; Fabio Cesar Gozzo4; Paulo Costa Carvalho3; 1Fiocruz - PR, Carlos Chagas Institute, Curitiba, Brazil; 2Research Center for Molecular Medicine of the Academy of Sciences, Vienna, Austria; 3Fiocruz - PR, Carlos Chagas Institute, Curitiba, Brazil; 4University of Campinas, Campinas, Brazil

TP 092  Optimization of LCMS acquisition settings for detection of crosslinked peptides; Ying Zhang1; Zhihui Wen1; Edward A Partlow2; Gunther Hollopeter1; Laurence Florens1; Michael P. Washburn1; 1Stowers Institute for Medical Research, Kansas City, MO; 2Department of Molecular Medicine, College of Veterinary Medicine, Cornell University, Ithaca, NY 14853; 3Department 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 Crowder1, 2; Vladimir Sarpe1; Daniel S. Ziemianowicz1, 2; Atefeh Rafiei3; David C. Schriemer1, 2, 3; 1Department of Biochemistry and Molecular Biology, University of California, Berkeley, CA; 2Robson DNA Science Centre, Arnie Charbonneau Cancer Institute, University of California, Berkeley, CA; 3Department of Chemistry, University of California, Berkeley, CA

TP 094  A crosslinking – mass spectrometry based multi-level integrative modeling approach to resolve the microtubule-doublecortin interaction; Atefeh Rafiei1; David C. Schriemer1; 1University of Calgary, Calgary, AB

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| TP 095 | Comprehensive Profiling of O-linked Glycans in Bovine Submaxillary Mucin; Yang Tang\(^1,2\); 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; Sivy (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 (\(\mu\)PACTM) 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 Glicosaminoglycans; 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\(^1,2,3\); Firas Kobeissy\(^4\); Raffaele Ferri\(^5\); 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 versus non-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 (\(\mu\)PACTM)-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 Q 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 Predelus1; Jon Amster1; 1University of Georgia, Athens, GA

TP 114  Relative Quantitation of HeLa Cell N-Glycans Using Deuterium Oxide Labeling for Global Omics Relative Quantification(DOLGOReQ); Jonghyun Kim1; Jua Lee2, 3; Dongtan Yin2, 3; Hyun Joo An2, 3; Tae-Young Kim1; 1Gwangju Institute of Science & Technology, Gwangju, South Korea; 2Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; 3Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea

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 Moorthy1; Christina Vedar1; Nicole R Zane1; Kevin J Downes1; Athena F Zuppa1; 1Children’s Hospital of Philadelphia, Philadelphia, PA

TP 116  LC-MS/MS-based enzyme assay for lysosomal storage disorders using dried blood spots; Ryuichi Mashima1; Mani Ohira1; Torayuki Okuyama1; 1National 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 Lin1, 2; Lidong He1; Lissa C. Anderson2; Archana M. Agarwa1, 3, 4; Alan L. Rockwood1, 3, 5; Chad R. Weisbrod2; Christopher L. Hendrickson2; Alan G. Marshall1, 2; 1Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; 2National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; 3University of Utah Health, Salt Lake City, UT; 4ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; 5Rockwood 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 Walker1; Yu Zhu1; Neloni Wijeratne1; 1Thermo Fisher Scientific, San Jose, CA

TP 119  Evaluation of automated quantitative analysis of the doubly charged glycated-hemoglobin by MALDI-TOF MS; Dennis JA Van Den Heuvel1; Andreas Schnapp2; Johan Scholten3; Archana M. Agarwa3, 4; Alan L. Rockwood1, 3, 5; Chad R. Weisbrod2; Christopher L. Hendrickson2; Alan G. Marshall1, 2; 1Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; 2National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; 3University of Utah Health, Salt Lake City, UT; 4ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; 5Rockwood Scientific Consulting, Salt Lake City, UT

TP 120  Fully automated LC-MS/MS method to assess DPD deficiency in Cancer treatment with 5-FU; Sascha Rexroth1; Doriane Toinon1; Tiphaine Robin1, 2; Stéphane Moreau1; Franck Saint-Marcoux1; 1Shimadzu Europa GmbH, Duisburg, Germany; 2Shimadzu Corporation, Kyoto, Japan; 3Shimadzu France, Paris, France; 4CHU 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 Laude1; Caitlyn Kanzian1; Kenneth Funk1; William Edgemon1; 1Genotox Laboratories, Austin, TX

TP 122  Monitoring of embryonic stem cell differentiation trajectories by intact cell mass spectrometry; Petr Vaňhara1, 2; Andreas Schnapp1; Lukáš Morá1, 2; Lukáš Pečinka4; Hana Kotasová1, 2; Vendula Pelková1; Josef Havell1, 4; Aleš Hampel1, 2; 1International Clinical Research Center, St. Anne's University Hospital Brno, Brno, Czech Republic; 2Faculty of Medicine, Masaryk University, Brno, Czech Republic; 3Shimadzu Europa GmbH, Duisburg, Germany; 4Faculty 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 Swiner1; George R. Durisek, II1; Abraham K. Badu-Tawiah1; 1The Ohio State University, Columbus, OH

TP 124  Rapid Intraoperative Detection of Isocitrate Dehydrogenase Mutations in Human Gliomas using a Miniature Mass Spectrometer; Hannah Marie Brown1; Fan Pu1; Mahua Dey2; James Miller2; Mitesh V. Shah2; Scott A. Shapiro2; Zheng Ouyang1, 3; Aaron A. Cohen-Gadol2; R. Graham Cooks1; 1Department of Chemistry and Bindley Biosciences Center, Purdue University, West Lafayette, IN; 2Department of Neurological Surgery, Indiana University School of Medicine, Indianapolis, Indiana; 3Montpellier university, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France; 4Montpellier university, CHU Montpellier, CMRR, Montpellier, France

TP 125  How to solve the disappearing methionine puzzle in new born screening?; Konrad Piotr Kowalski1; Tomasz Bienkowski1, 3; Anna Kolodyńska-Goworek2; Katryna Poleć-Pawlak2, 4; Anna Czyż2; 1Masdiag Sp. z o.o., Warszawa, Poland; 2Masdiag Sp. z o.o., Warszawa, Poland; 3MS Ekspent Sp. z o.o., Gdańsk, Poland; 4Warsaw University of Technology, Warszawa, Poland

TP 126  MALDI-TOF IP-MS quantification of plasma amyloid peptides in Alzheimer’s disease; Jerome Vialaret1; Jana Kindermans1; Sylvain Lehmann1; Audrey Gabelle2; Christophe Hirtz1; 1IRMB, Univ Montpellier, INSERM, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France; 2Montpellier 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. DeHoog1; Monica Lin1; Jialing Zhang1; John Lin1; Kirtan Brahmbhatt2; Wendong Yu2; Robert Tibshirani3; James Suliburk2; Livia S Eberlin1; 1University of Texas at Austin, Austin, TX; 2Baylor College of Medicine, Houston, TX; 3Stanford 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 Auger1; Pierre Picard1; Jean Lacoursière1; 1Phytonix Technologies, Quebec, QC

TP 129  Determination of sex hormones in human serum and plasma using a LC/TQ medical device; Suparna Mundodi1; Xiaoli Dong1; 1Agilent Technologies, Santa Clara, CA

TP 130  Deep, reproducible and high-throughput FFPE analyses: moving toward large-scale clinical omics applications; Matthew Willetts1; Christopher Swift1; John P Wilson2; Shourjo Ghose2; 1Bruker, Billerica, MA; 2Bruker Daltonics, Billerica, MA; 3Protifi, LLC, Farmingdale, NY

TP 131  Steroid Conjugates: an aid for a comprehensive insight of endocrine health; Ahmed Najar1; Melissa Bennett1; George Gillson1; 1LifeLabs, 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 Garza1; Jialing Zhang1; Marta Sans1; Rachel J DeHoog1; Mary King1; Alena Bensussan1; Michael F Keating1; John Lin1; Stacey A Carter2; Alastair Thompson2; Elizabeth Bonefas2; Chandandeep Nagi2; Chris Pirko2; Kirtan Brahmbhatt2; James Suliburk2; Livia S Eberlin1; 1University of Texas, Austin, TX; 2Baylor College of Medicine, Houston, TX

TP 133  Liquid Chromatography-Mass Spectrometry Determination of Atorvastatin in Eye Vitreous Humor of Diabetic Patients; Kingsley Donkor1; Taran Main1; Colten Wendel2; Zhi Chao Guo1; 1Thompson Rivers University, Kamloops, BC; 2St. Paul's Hospital, Vancouver, BC

TP 134  Thin film molecularly imprinted polymers (MIPs) for selective and high throughput analysis of biological samples; Fereshteh Shahhoseini1; Evan A. Langille2; Ali Azizi2; Carlos A. Bazan2; Christina Bottaro2; 1Memorial University of Newfoundland, St. John’s, NL; 2Memorial University, St. John's, NL

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

TP 138  Plasmodium chaperonin TCP-1 identified as target of antihistamine clemastine using energetic-based proteomics studies; Baiyi Quan1; Kuan-Yi Lu1, 2; Kayla R. Sylvester2; Tamanna Srivastava1; Michael C. Fitzgerald1; Emily R. Derbyshire1, 2; 1Department of Chemistry, Duke University, Durham, NC; 2Department 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 Häbe1; Frank Runge1; Chang Liu2; Tom R Covey2; Andreas Harald Luippold1; 1Boehringer Ingelheim, Drug Discovery Sciences, Biberach an der Riss, Germany; 2SCIEX, 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 Wang1; Miao He1; Bo Wen1; Manjunath Pai1; Hebao Yuan1; Duxin Sun1; 1University of Michigan, Ann Arbor, MI

TP 141  Development of a clinically relevant dosing (CRD) approach in mice for studying acquisition of antibiotic resistance; Xiaoyu Wang1; Erika Serrano Diaz1; Laura Coughlin1; Marguerite Monogue1; Andrew Y. Koh1; Erdal Toprak1; 1UT Southwestern Medical Center, Dallas, TX

TP 142  Trapping of Reactive Acyl Glucuronides by a Protein Surrogate for a Tool for the Assessment of Potential Idiosyncratic Toxicities; Jian Yu1; Heng Keang Lim2; Mary Jo Wildey2; David G Mclaren1; 1Drug Metabolism and Pharmacokinetics, Discovery Sciences, Janssen Pharmaceutical companies of Johnson & Johnson, Springhouse, PA; 2Drug 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; Xiujian Wen1; Kiersten Tovar1; Lucien Ghislain2; Chang Liu3; Kenneth Ellsworth1; Mary Jo Wildey1; David G Mclaren1; 1Merck & Co., Kenilworth, NJ; 2Beckman Coulter Life Sciences, San Jose, CA; 3SCIEX, Concord, Ontario
TUESDAY POSTERS (TP) Pages 45-85 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

TP 144  
**Hepatocyte Spheroids as a Viable in vitro Model for Recapitulation of Complex in vivo Metabolism**  
Pathways of Loratadine in Humans; Silvi Chacko\(^1\); Van T Ly\(^2\); Lisa J. Christopher\(^6\); Jingping Gan\(^3\); \(^1\)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)**; Can Ozbal\(^1\); William Albino Lamarr\(^1\); Ian Mckenna\(^3\); Arrin Katz\(^1\); \(^1\)PureHoney Technologies, Inc., Billerica, MA

TP 146  
**Intact Protein Analysis Enables Pharmacokinetic/Pharmacodynamic Profiling of Covalent Drug Candidates**; Md Amin Hossain\(^1\); Rutali R. Brahme\(^1\); Jakal Amin\(^1\); Durgalakshimi 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\(^1\); 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**; Thomas Lloyd\(^1\); Eduardo E. Lopez\(^2\); \(^1\)Worldwide Clinical Trials, Austin, TX

TP 148  
**Mass Spectral Characterization of Bilirubin by Electrospray Ionization, H/D Exchange, and Multiple Stage Mass Spectrometry**; Stephen U Bowlin\(^1\); 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**; Catalina Suarez\(^1\); Qi Wu\(^1\); Yongying Jiang\(^1\); \(^1\)UT MD Anderson Cancer Center, Houston, TX

**ENVIRONMENTAL: GENERAL I**

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**; Beibei Huang\(^1\); 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**; Taylor J. Glattke\(^1\); 2; Martha L. Chacon-Patiño\(^3\); 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\(^3\); Feng Qin\(^1\); \(^1\)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 Effortless**; Joseph Mick\(^1\); Andrea Moberly\(^1\); \(^1\)Heritage Research Group, Indianapolis, IN

TP 154  
**Statistical approach for the analysis of emerging contaminant (CECs) in complex water samples during treatment processes**; Zsuzsanna Varga\(^1\); 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**; Albert T Lebedev\(^1\); 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**; Jiancheng Yu\(^1\); 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**; Rai Matat\(^1\); Andy Ommen\(^1\); \(^1\)MilliporeSigma, Laramie, WY

TP 158  
**Proteomics analysis of whole-body responses in medaka (Oryzias latipes) exposed to benzalkonium chloride**; Young Sang Kwon\(^1\); 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**; Huiyu Dong\(^1\); 2; Amy A. Cuthbertson\(^1\); 3; Susan D. Richardson\(^1\); \(^1\)Bristol-Myers Squibb, Princeton, NJ; \(^2\)Bristol-Myers Squibb Company, Princeton, NJ

TP 160  
**Testing the Removal of Microcystins from Water Using a Column Packed with Rice Husk**; Sharmila I Thenuwar\(^1\); David Balu-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 Llewellyn1; John Wilkinson2; Brett Sallach2; Ramón González-Méndez2; Olaf Schelbner2; Christina Jacob1; Martin Jech1; 1ThermoFisherScientific, Hemel Hempstead, United Kingdom; 2York University, York, United Kingdom; 3York University, York, United Kingdom; 4University of California, Los Angeles, Los Angeles, CA; 5Gladstone Institutes, San Francisco, 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 Pike1; Jennifer A. Faust1; Paul L. Edmiston2; Jillian Morrison3; 1The College of Wooster, Wooster, OH

TP 164 Demonstrating Improvements in PFAS Sensitivity Using a Microflow LC Approach for the EPA 537 Panel; Katherine Hyland1; Karl Oetjen2; Simon Roberts3; Diana Tran4; 1SCIEX, Redwood City, CA; 2SCIEX, Redwood Shores, California 1201; 3SCIEX, Redwood Shores, CA

TP 165 Evaluating Removal Efficiency of CECs in Decentralized Wastewater Treatment Technologies using GCxGC/TOF-MS; Jade L Johnson1; Eunha Hoh1; Natalie Mladenov2; Nathan G Dodder1; William H Richardot1; Lauren Steinberg2; 1School of Public Health, San Diego State University, San Diego, CA; 2Department 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, Heuksae-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-Patino1, 2; Sydney F. Niles1, 2; Taylor J. Glattke1, 2; Amy Mckenna1, 2; Donald F. Smith1, 2; Alan G. Marshall1, 2; Christopher L. Hendrickson1, 2; Ryan P. Rodgers1, 2; 1Florida State University, Tallahassee, FL; 2National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL

TP 168 Real time analysis of toluene degradation in a dielectric barrier discharge plasma; Michel Heninger1; Essyllt Louarn1; Helene Mestdagh1; Joel Lemaire1; Stephane Pasquiers1; Nicole Blin-Simian2; 1ICP, CNRS, Université Paris Saclay, Orsay, France; 2LPGP, 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 Aziz1; Danielle C. C. Westerman1; Amy A. Cuthbertson2; Sam Putnam2; John L. Ferry1; Susan D. Richardson1; Leanne Powers2; Michael Gonsior3; 1University of South Carolina, Columbia, SC; 2University of California, Berkeley, Berkeley, CA; 3University 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 Monaghan1; Lindsay Hounjet1; Stanislav R. Stoyanov1; John V. Headley1; Kerry M. Peru1; Christopher G. Gill1; Erik T. Krogh1; 1Applied Environmental Research Laboratories, Chemistry, Vancouver Island University, Nanaimo, BC; 2Natural Resources Canada, Devon, AB; 3Environment 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 Organtini1; Stuart Oehrle1; Kenneth Rosnack1; 1Waters Corporation, Milford, Massachusetts

TP 172 Detection and/or quantification of modified RNA by LC-MS/MS: a new tool of discovery of a cancer biomarker; Aurore Attina1; Jerome Vialaret1; Amandine Amlaric2; Hélène Guillorit2; Amandine Bastide2; Sébastien Relier2; Eric Rivals2; Emmanuelle Samalin2; Evelyne Crapez2; Sylvain Lehmann1; Alexandre David2; Christophe Hirtz1; 1IRMB, Univ Montpellier, INSERM, CHU Montpellier, (LBPC-PPC), Montpellier, France, Montpellier, France; 2Institute for Functional Genomics, Montpellier, France; 3Laboratory of Computer Science, Robotics and Microelectronics of Montpellier, Montpellier, France; 4Cancer 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; Seunjeon Na1; Eunok Paek1; 1Hanyang University, Seoul, South Korea

TP 174 Targeted Proteomic Analysis for Interrogating the Epitranscriptomic Regulations of Small GTPases; Yen-Yu Yang1; Ming Huang1; Yinsheng Wang1; 1UC Riverside, Riverside, CA

TP 175 Global ubiquitination profiling of HIV-1-infected cells reveals mechanisms of host cellular chromatin remodeling; Jeffrey Johnson1; Donna Li2; Oliver Fregoso3; Nevan Krogan4, 5; 1Icahn School of Medicine at Mount Sinai, New York, NY; 2University of Wisconsin, Madison, WI; 3University of California, Los Angeles, Los Angeles, CA; 4University of California San Francisco, San Francisco, CA; 5Gladstone Institutes, San Francisco, CA
TUESDAY POSTERS (TP) Pages 45-85 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

TP 176  
Systematic investigation of PRMT6 substrate recognition reveals broad specificity with a preference for basic and bulky residues; Joshua J Hamey1; Sinja Rakow2; Caoline Bouchard2; Uta Maria Bauer; Marc R Wilkins1; Gene Hart-Smith1; 1School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia; 2Institute for Molecular Biology and Tumor Research (IMT), Philippus-University Marburg, Marburg, Germany; 3Department 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; Mandy W. M. Wong1; Ryan J. Separovich1; Marc R Wilkins1; 1Systems Biology Initiative UNSW, Sydney, Australia

TP 178  
The role of upstream phosphorylation in the regulation of histone methylation; Ryan J. Separovich1; Joshua J Hamey1; Marc R Wilkins1; 1School 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; Christopher R. Beekman1; Rahul Pawar1; 1U.S. Food and Drug Administration, College Park, MD

TP 180  
Atmospheric Solid Analysis Probe mass spectrometry for food compliance screening: oregano authenticity case study; Tito Damiani1; Nicola Dreolin2; Sara Stead2; Chiara Dall'asta1; 1University of Parma, Parma, Italy; 2Waters Corporation, Wilmslow, United Kingdom

TP 181  
Potential of trapped-ion-mobility UHPLC-QTOF in food authenticity studies: characterization of co-eluting secoiridoid isomers found in Greek extra virgin olive oil; Sofia K. Drakopoulou1; Dimitrios E Damalas1; Nikolaos S. Thomaidis1; Carsten Baessmann2; 1National and Kapodistrian University of Athens, Athens, Greece; 2Bruker 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 Stead1; Emmanuelle Claude1; Christopher Henry1; Steve Preece1; Kenneth Rosnack2; 1Waters Corporation, Wilmslow, United Kingdom; 2Waters Corporation, Darlington, PA

TP 183  
Investigations into Small Molecule Pesticide Protomers and Conformers Using Linear and Cyclic Ion Mobility Separators; Mike_mccullagh@waters.com Mccullagh1; Martin Palmer1; Jakub Ujma1; Emma Marsden-Edwards1; Séverine Gosciny1; 1Waters Corporation, Wilmslow, United Kingdom; 2Sciensano, Brussels, Belgium

TP 184  
Real-time monitoring of frying fumes composition using proton transfer reaction mass spectrometry; Tomasz Majchrzak1; Wojciech Wojnowski1; Agnieszka Głowińka-Różyńska1; Andrzej Wasik1; 1Gdansk University of Technology, Department of Analytical Chemistry, Gdansk, Poland; 2Gdansk 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; Justin T Marsh1; Charles Yang2; Philip E Johnson3; 1University of Nebraska Lincoln, Lincoln, NE; 2ThermoFisher Scientific, San Jose, CA; 3University of Nebraska-Lincoln, Lincoln, NE

TP 186  
An MRM-based Method for Quantitative Analysis of Functional Carotenoids in Biological and Food Samples; Zhe Sun1; Jie Xing1; Hui Zhang1; Nicole Jia Min Chen2; Zhaoqi Zhan1; 1Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; 2National University of Singapore, Singapore, Singapore

TP 187  
LC-QTOF-MS identification of rabbit-specific peptides for meat species control in meat products; Anna Stachniuk1; Agata Sumara1; Magdalena Montowska2; Emilia Formal1; 1Medical University of Lublin, Lublin, Poland; 2Poznan University of Life Sciences, Poznan, Poland

TP 188  
Selection of peptide targets for species-independent quantitation of fish allergens; Justin T Marsh1; Charles Yang2; Philip E Johnson3; 1University of Nebraska Lincoln, Lincoln, NE; 2Thermo Fisher Scientific, San Jose, CA; 3University of Nebraska-Lincoln, Lincoln, NE

TP 189  
Beer processomics: Untargeted profiling of volatile and nonvolatile compounds throughout the production of a single hop, single malt (SMaSH) beer; Lynn E. Marsh1; Adrianna R. Losquadro1; Ashleigh E. Outhous1; Samuel A. Morton1; Steven Harper1; Christine A. Hughey1; 1James Madison University, Harrisonburg, VA

TP 190  
Rapid UHPLC Identification of Anthocyanins from Different Varieties of Berries using High Resolution-QTOF-Mass spectrometry; Jashbir Singh1; Jayashan Adhikari2; G. K. Jayaprakash2; Bhimanagouda S. Patil2; 1Texas A & M University, College Station, TX; 2Waters Corporation, Darlington, PA

TP 191  
Aquaculture Proteomics for the Evaluation of Antibacterial Feed on Paralichthys Olivaceus; Jihoon Shin1; Min-kyu Youn1; Miseon Jeong1; Junghoon Kang1; Youngjin Kim1; Wonryeon Cho1; 1Wonkwang University, Iksan, South Korea
TUESDAY POSTERS (TP) Pages 45-85 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

GLYCOPROTEINS II
TP 193-209

TP 193  Spot the Differences: Assessing site-specific glycosylation similarity between influenza A virus variants with statistical certainty; Deborah Chang1; William E Hackett2; Joshua A Klein2; Joseph Zaia1,2; 1Boston University School of Medicine, Boston, MA; 2Bioinformatics Program, Boston University, Boston, MA

TP 194  Characterization of High Mannose and Phosphorylated High Mannose Glycosylation Sites in Hybrid β-Hexosaminidase (HexM); Taylor Battellino1; Tyler Tran1; Duc Minh Nguyen1; Graeme Berzini1; Oleg Krokhin1; Brian Mark1; Helene Perreault1; 1University of Manitoba, Winnipeg, MB

TP 195  Enrichment Assisted Identification of Glycosylated Neuropeptides in Crustaceans; Ashley Phetsanathad1; Lingjun Li1,2; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2School of Pharmacy, University of Wisconsin-Madison, Madison, WI

TP 196  Glycosylation Patterns in Neoplastic Biomarker Alpha Fetoprotein in Pathologic Human Serum Samples; Mark M Kushnir1; YiFei K Yang1,2; 1ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; 2University of Utah, Salt Lake City, UT

TP 197  Optimization of glycopeptide analysis workflow using Chinese Hamster Ovary Cells; Hsiang-En Hsu1; Raghovatha Chaerkady1; Matthew Glover1; Gargi Roy1; Sonja Hess1; 1R&D, AstraZeneca, Gaithersburg, MD

TP 198  Evaluation of O-glycosylation via O-glycan specific Proteolysis, LC-MS and Rapid Data Processing; Charles Nwosu1; Lei Wang2; Yang Wang2; Chris Barton2; 1Takeda Pharmaceuticals International Co, Cambridge, MA; 2Takeda 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 Kim1; Marshall Bern2; David C. Dallas1; 1Oregon State University, Corvallis, OR; 2Protein Metrics Inc., Cupertino, CA

TP 200  Enrichment-free O-glycoproteome based on Trapped Ion Mobility Q-TOF; Xue Sun1; Wenmin Tian1; Jianhui Cheng2; Ning Chen3; Yang Chen1; Catherine C L Wong1; 1Center for Precision Medicine Multi-Omics Research, Peking University, Beijing, China; 2Department of Chemistry, University of British Columbia, Vancouver, BC; 3Bruker Daltonics, Beijing, China

TP 201  Quantitative O-glycosylation characterization in fetuin by hot electron capture dissociation, detection of more than fifty O glycopeptides; Takashi Baba1; Suya Liu1; Pavel Ryumin1; 1SCIEX, Concord, ON

TP 202  Improving UPLC/MS N-glycosylation analysis of disulfide-rich fusion proteins through optimization of sample preparation conditions; Ximo Zhang1; Mauro Sassi2; Erika Birolo2; Paolo Felici3; Nunzio Sepe3; Antonio Datola4; Robert Birdsall1; Ying-Qing Yu1; 1Waters Corps, Milford, MA; 2Merck 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 Chandler1; Vanessa L Stahl1; Bach-Cuc Nguyen2; Maria A Kukuruzinska2; Catherine E. Costello1; 1Center for Biomedical Mass Spectrometry, Department of Biochemistry, Boston University School of Medicine, Boston, Massachusetts; 2Department of Translational Dental Medicine, Boston University School of Dental Medicine, Boston, Massachusetts

TP 204  Large Scale Analysis of Sialic Linkage Isoomers from Intact Glycopeptides Reveals Structural Diversity; Jonathan C. Trinidad1; Kathleen T. Grassmyer1; Xuyao Zeng1; David E. Clemmer1; 1Indiana University, Bloomington, IN

TP 205  Optimizing the duration of hydrazine hydrate chemical deglycosylation for MS analysis of mucin-type O-linked glycans; Bryan E Hettick1; Elyssa S. Gallagher1; 1Baylor University, Waco, TX

TP 206  RAMZIS: a bioinformatic tool for rigorous assessment glycoprotein similarities from LC-tandem mass spectrometric data; William E Hackett1; Deborah Chang2; Luis Carvalho3,4; Joseph Zaia1,2; 1Boston University, Boston, MA; 2Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; 3Department of Mathematics, Boston University, Boston, MA; 4Bioinformatics 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 Bell1; Eric D Dodds1; 1University of Nebraska-Lincoln, Lincoln, NE

TP 208  Comprehensive N- and O-glycosylation characterization of multiple CHO host cell lines using HILIC-GIG method; Qiong Wang1; Shuang Yang2; Tiexin Wang1; Michael J. Betenbaugh1; John Cipollo2; Yuan Tian2; 1JHU Chemical Engineering Department, Baltimore; 2FDA Laboratory for Bacterial Polysaccharides, Silver Spring, Maryland

TP 209  An automated MS data workflow enabling targeted, site-specific glycosylation monitoring in continuous biopharmaceutical manufacturing; Bertacconi Diego; Merck KGaA, Corsier-sur-Vevey, Switzerland
All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.
**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; Qinying Yu; Pamela R. Westmark; Cara J. Westmark; Lingjun Li; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; Department of Neurology, University of Wisconsin-Madison, Madison, WI; 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; Geert Baggerman; Centre for Proteomics, Antwerpen, Belgium; 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; Andy Weiss; Kelli L Boyd; Nathan Heath Patterson; Jeffrey M Spraggins; Richard M Caprioli; Todd Westmark; Thomas P Westmark; Department of Infectious Diseases and Immunology, Vanderbilt University, Nashville, TN; Department of Surgery, Vanderbilt University, Nashville, TN; Department of Pathology, Vanderbilt University, Nashville, TN; Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; Department of Phycology and Immunology, School of Medicine, Vanderbilt University, Nashville, TN; Department of Molecular Biology, Vanderbilt University, Nashville, TN; Department of Pharmacology, Vanderbilt University, Nashville, TN; 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; Marcella Cardoso; John Q Lin; Charlotte Hueblauer; Geisilene R. P. Silva; Marcos N. Eberlin; Livia S. Eberlin; Sophie F. M. Derchain; Andrea M. Porcarli; Laboratory of Multidisciplinary Research, São Francisco University, Bragança Paulista, Brazil; Department of Gynecological and Breast Oncology, Women's Hospital (CAISM), Faculty of Medical Sciences, State University of Campinas (UNICAMP), Campinas, Brazil; Department of Chemistry, University of Texas at Austin, Austin, Texas; Medical University of Graz, Graz, Austria; 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; Mayuka Kosugi; Naohiko Nakamura; Takashi Nirasawa; Ryo Kajita; Etsuro Hatano; Shugo Ueda; Hiroaki Terajima; Shinji Uemoto; Masaya Ikegawa; Kitano Hospital, The Tazuke Kofukai Medical Research Institute, Osaka, Japan; Department of Surgery, Graduate School of Medicine, Kyoto University, Kyoto, Japan; Department of Life and Life Sciences, Faculty of Life and Medical Sciences, Doshisha University, Kyotanabe, Japan; Bruker Japan K.K., Yokohama, Japan

**TP 215**
**Dissecting Rostral Migratory Stream (RMS) through MALDI-Imaging Mass Spectrometry on murine olfactory deprivation model:** Daiki Kameyama; Takashi Nirasawa; Ryo Kajita; Nobuto Kakuda; Masaya Ikegawa; Faculty of Life and Medical Science, Department of Life and Medical Systems, Doshisha University, Kyotanabe City, Japan; 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; Takashi Tsuji; Mizuki Ishida; Takashi Nirasawa; Ryo Kajita; Hatsue Ishibashi-Ueda; Hidetoshi Masumoto; Kenji Minatoya; Masaya Ikegawa; Doshisha University, Kyotanabe, Japan; Kyoto University, Kyoto, Japan; 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; Lucia Martin-Saiz; Albert Maimó-Barceló; Javier Martin; Juan J. Gutiérrez; Joan Bestard-Escalas; Daniel H. López; Sam Khorrami; Marcelo Garcia; Tom K. Abban; Matthew E. Openshaw; Gwendolyn Barceló-Coblijn; José A. Fernández; Shimadzu, Manchester, United Kingdom; Department of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena s/n, 48940, Spain; Research Unit, Hospital Universitari Son Espases, Institut d’Investigació Sanitària Illes Balears(IdISBa), Palma, Spain; Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain

**TP 218**
**Mass Spectrometry Imaging to Differentiate between Pancreatic Adenocarcinoma and Cholangiocarcinoma:** Christine Bollwein; Alice Ly; Juliana Goncalves; Sören-Oliver Deininger; Wilko Weichert; Kristina Schwamborn; Institute of Pathology, Technical University Munich, Munich, Germany; Bruker Daltonik GmbH, Bremen, Germany

**TP 219**
**High Resolution Imaging Mass Spectrometry of Human Donor Eyes with Retinal Pathology:** David M. G. Anderson; Ankta Kotnala; Jarod A. Fincher; Jeffrey D. Messinger; Nathan Heath Patterson; Jeffrey M Spraggins; Christine A. Cucicio; Kevin L. Schey; Vanderbilt University, Department of Biochemistry, Nashville, TN; University of Alabama at Birmingham, Birmingham, AL

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TP 220  Helicobacter pylori-induced Molecular Alterations in Gastric Tissue Visualized by Imaging Mass Spectrometry; Michelle Reyzer1; Aung Soe Lin1; Jeff Shaw1; Ankita Kotnala1; Michael Tuck1; Jennifer Harvey1; Maria B. Piazzuelo1; Kevin L. Schey1; Timothy Cover1; Richard M Caprioli1; 1Vanderbilt University, Nashville, TN

TP 221  Comparative Ultra-high Resolution Imaging MS Reveals Lipid and Fatty Acid Dyshomeostasis in a 3K a-Synuclein Parkinson’s-like Mouse Model; Madison H. Mcminn1, 2; Silke Nuber2; Walid Abdelmoula2; Sylwia A. Stopka2; Dennis Selkoe4; Jeffrey N. Agar1; Nathalie Y. R. Agar3, 4, 5; 1Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; 2Department of Neurosurgery, Brigham and Women’s Hospital, Harvard Medical School, Boston, MA; 3Ann Romney Center for Neurologic Diseases, Department of Neurology, Brigham and Women’s Hospital and Harvard Medical School, Boston, MA; 4Department of Radiology, Brigham and Women’s Hospital, Harvard Medical School, Boston, MA; 5Department 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 Ajasin1; Brendan Pradeaux1; Eliseo Eugenin1; 1University 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 Popov1, 2; Evgeniy Zhvansky1; Danill Ivanov1; Stanislav Pekov1; Anatoly Sorokin1; Vsevolod Shurkhay1, 2; Denis Zavorotnyuk1; Pavel Nikitin2; Alexander Potapov2; Eugene (evgeny) Nikolaev3; 1Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 2N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; 3Skolkovo 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 Tanaka1; Hiroki Yamashita1; Takashi Nirasawa2; Ryo Kajita2; Katsutoshi Taguchi3; Masaki Tanaka3; Takayuki Kondo4; Nobuto Kakuda1; Masaya Ikegawa1; 1Doshisha University, Kyoto, Japan; 2Broker Japan K.K., Yokohama, Japan; 3Department of Anatomy and Neurobiology, Graduate School of Medical Science, Kyoto Prefectural University of Medicine, Kyoto, Japan; 4Kansai Medical University Medical Center, Hirakata, Japan

TP 225  AP-SMALDI-MSI of Cryptosporidium parvum and Neospora caninum-infected cells and tissue; Nils Anschütz1; Stefanie Gerbig1; Camilo Larrazabal1; Juan Velez2; Liliana Silva3; Carlos Hermosilla4; Anja Taubert5; Bernhard Spengler1; 1Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany; 2Institute 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 Piga1; Giulia Capitoli1; Francesca Clerici1; Alia Mahajneh1; Virginia Brambilla2; Vanna Denti1; Andrew Smith1; Stefania Galimberti1; Fulvio Magni1; Fabio Pagni1; 1University of Milano – Bicocca, Proteomics and Metabolomics platform, School of Medicine and Surgery, Vedano al Lambro, Italy; 2University of Milano – Bicocca, School of Medicine and Surgery, Pathology Section, San Gerardo Hospital, ASST Monza, Italy; 3University 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 Shrestha1; Anthony Midy1; Hernandez Olivos1; Long Yuan2; Zhiyun Li2; Jia Peng2; Qihong Zhao2; Qin Ji2; 1Waters Corporation, Beverly, MA; 2BMS Co., Princeton, NJ

IMAGING MS: SMALL MOLECULES

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 Claude1; Mark Towers1; Rene Lafort2; Ian D Wilson3; Robert Plumb1; 1Waters Corporation, Wilmslow, United Kingdom; 2Sorbonne Université, Campus Pierre et Marie Curie, IBPS-BIOSIPE, Paris, France; 3Division of Systems Medicine, Department of Metabolism, Digestion and Reproduction, Imperial College London, South Kensington, United Kingdom; 4Waters 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 Larson1; Elias P Rosen1, 2; Matthew R Lockett1, 3; Gary L Glish1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2UNC Eshelman School of Pharmacy, Chapel Hill, NC; 3Lineberger 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-Diaz1; Arlet M. Acanda De La Rocha1; Jeremy W. Chambers1; Francisco Fernandez-Lima1; 1Florida International University, Miami, FL; 2Florida International University, Miami, Florida

TP 231  Alterations in lipid profile of a depression model detected by MALDI-imaging mass spectrometry; Jong Bok Seo1; Eui-Gil Jung1; Hee-Jung Kim1; Bong June Yoon1; Jinnyoung Choi2; 1Korea Basic Science Institute, Seoul, South Korea; 2Korea University, Seoul, South Korea; 3Bruker Korea, Seongnam, South Korea
TP 233  Rapid discrimination of Panax ginseng in different growing years using DESI-MS imaging coupled with chemometrics; Yuangui Yang1; Yanchao Shi2; Yingbo Yang3; Kate Yu4; Ming Yuan2; Zhengtang Wang5; Li Yang6; 1Shanghai University of Traditional Chinese Medicine, Shanghai, China; 2Waters Corporation Shanghai Science & Technology Co Ltd, shanghai, China; 3Kanion Pharmaceutical Co., Ltd, Jiangsu, Lianyungang, China; 4Shanghai University of Traditional Chinese Medicine, shanghai, China

TP 234  Mass Spectrometry Imaging in Cesium Mapping for Thermochemical Ablation: Correlation with Dual-Energy Computed Tomography; Emily A. Thompson1; Dodge L. Baluya1, 2; A. Colleen Crouch1; Megan C. Jacobsen1; Rick R. Layman1; Elizabeth M. Whitley1; Erik N.K. Cressman1; 1MD Anderson Cancer Center, Houston, TX; 2Washington State University, Pullman, WA

TP 235  New data flow model for rapid automated processing of large volumes of LC/UV/MS data; Richard Lee1; Andrey Panaramov3; Vladislav Solomatov1; Eugene Volopianov1; 1ACD/Labs, Toronto, ON

TP 236  high-throughput labeled LC-MS/MS data normalization and automated reporting; Joris Van Houtven1, 2, 3; Evelyne Maes1; Kris Laukens5; Geert Baggerman2, 3; Jef Hooyberghs2; Dirk Valkenborg1, 2, 3; 1Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Data Science Institute, Hasselt University, Hasselt, Belgium; 2Flemish Institute for Technological Research (VITO), Mol, Belgium; 3Centre for Proteomics, Antwerpen, Belgium; 4AgResearch, Christchurch, New Zealand; 5Biomina, Antwerpen, Belgium

TP 237  A new version of the PRIDE database including a new interactive website and Restful API; Suresh C Hewapathirana1; Jingwen Bai1; Chakradhar Bandla1; David Garcia-Seisedos2; Selvakumar Kamatchinathan1; Deepti J. Kundu1; Juan Antonio Vizcaino1; 1European Bioinformatics Institute, Cambridge, United Kingdom

TP 238  New Functionalities in proteoX Facile Integration of Data Normalization and Informatic Analysis for Quantitative Proteomic Workflows Using Tandem Mass Tags; Qiang Zhang1; R Reid Townsend1; 1Washington University School of Medicine, St. Louis, MO

TP 239  Towards a Computational Workflow for the Analysis of DOM Fragmentation Data; Muhammad Usman Tariq1; Dennyx Leyva3; Francesco Fernandez-Lima3; Fahad Saeed1; 1Florida International University, Miami, FL

TP 240  LC-MS/MS system suitability evaluation with automated data processing for protein analysis in a regulated environment; Wencheng Ge1; Bhavin Patel1; 1Thermo Fisher Scientific, Rockford, IL

TP 241  Updates on Philosopher: a complete toolkit for both conventional and open search-based shotgun proteomics data analysis; Felipe Da Veiga Leprevost1; Sarah E. Haynes1; Fengchao Yu1; Avinash K. Shanmugam1; Dattatreya Mellacheruvu1; Hui-Yin Chang1; Dmitry M. Avtonomov1; Andy Kong1; Alexey I. Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

TP 242  A data analysis pipeline for quality control and differential expression analysis of quantitative proteomics; Frank Koopmans1; Miguel A Gonzalez-Lozano1; August B Smit1; Ka Wan Li1; 1VU university, Amsterdam, Netherlands

TP 243  MassIVE: bridging the gap between data and discovery through large-scale reanalysis; Jeremy Carver1; Julie Wertz1; Benjamim Pullman1; Nuno Bandeira1; 1UCSD, La Jolla, CA

TP 244  SimpLiFi: a GPU-driven data-to-meaning analytics engine to bring omics understanding to all; Darryl J. Pappin1; 2; John Wilson1; 1ProtiFi, LLC, Farmingdale, New York; 2Cold Spring Harbor Laboratory, COLD SPRING HARBOR, New York

TP 245  Production and Generation of Proteogenomics Databases using PyPGATK; Husen M. Umer1; Yafeng Zhu2; Enrique Audain1; Janne Lehtii1; Rui Branca1; Yasset Perez-Riverol2; 1Department of Oncology-Pathology, Science for Life Laboratory, Karolinska Institutet, Stockholm, Sweden; 2Department of Genetics, Harvard Medical School, Boston, MA 02115; 3Department of Congenital Heart Disease and Pediatric Cardiology, Universitätsklinikum Schleswig–Holstein Kiel, Kiel, Germany; 4European 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; Chen Hao1; Xiaoxu Zhou2; Meng Luo2; Tiansheng Zhu2; Tiannan Guo2; Lu Li2; 1Westlake University, hangzhou, China; 2Westlake University, Hangzhou, China

TP 247  "TimsPy": access timsTOF Pro data easily from Python; Mateusz Krzysztof Lacki1; Sven Brehmer2; Ute Distler1; Stefan Tenzer1; 1University Medical Center, Johannes Gutenberg University, Mainz, Germany; 2Bruker Daltonik GmbH, Bremen, Germany

TP 248  Scalability Redefined: A new workflow in Spectronaut to analyze 10'000+ raw files on a desktop workstation; Oliver M. Bernhardt1; Jakob Vowinckel1; Tejas Gandhi1; Lukas Reiter1; 1Biognosys AG, Schlieren, Switzerland
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TP 250
Mass Spectrometer Observing Lunar Operations (MSolo); Roberto Aguilar1; Janine E. Captain1; Jacqueline W. Quinn1; Julie E. Kleinhenz2; Kenneth Wright6; Jorge Andres Diaz5; James D. Fox4; Jaime Winfield5; Peter Santariello3; Kris Zaczyn4; Zachary Mank5; Gale Paulsen1; 1National Aeronautics and Space Administration, Kennedy Space Center, FL; 2National Aeronautics and Space Administration, Johnson Space Center, TX; 3INFICON, Syracuse, NY; 4Honeybee Robotics, Altdadena, CA

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Hyperthermal Ion Beam Deposition Using a Rotating Wall Mass Analyzer; Pei Su1; Michael Forrester Espenship1; Julia Laskin1; 1Purdue University, West Lafayette, IN

TP 252
An optimized PTR3-TOFMS instrument for high-sensitivity and high-resolution analysis in atmospheric research and environmental chemistry; Tobias Reinecke1; Alfons Jordan1; Markus Leiminger1; Stefan Feil1; Christian Lindinger1; Lukas Märk1; Philipp Sulzer1; 1IONICON Analytik GmbH., Innsbruck, Austria

TP 253
Ion Manipulation Effects Inside a Digitally Driven Quadrupole; Margaret E. Reece1; Adam P. Huntley1; Conner F. Bailey1; Sumeet Chakravorty1; Peter T.A. Reilly1; 1Washington State University, Pullman, WA

TP 254
Computational Evaluation of Sine and Rectangular Wave Mass Filter Acceptance and Transmittance Influenced by Developing Fields; Adam P Huntley1; Peter T. A. Reilly1; 1Washington State University, Pullman, WA

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A novel ion optical device to improve duty cycle of a Q-TOF mass spectrometer; Xiaojing Zhang1; Wenjian Sun1; Lin Liu1; Leping Huang1; 1Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China

TP 256
Construction of a miniature digital rectilinear ion trap (DRIT) mass spectrometer; Han Bin Oh1; Jae-ung Lee1; Igor Filippov2; 1Soong Unv. Dept. of Chemistry, Seoul, South Korea; 2Auckland Unv. Dept. of Physics, Auckland, New Zealand

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Fundamental Principles and Performance for a Low Vacuum Mass Spectrometer; Yiming Lin1; Wenjian Sun1; Qiao Jin1; Hongbing Cheng1; 1Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China

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TP 261
A soft ionization source for generating, storing, and ejecting positive and negative ions; Qinghao Wu1; Xiaofeng Zhao1; 1IonX 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; Abraham L. de la Cruz Hernandez1; Daniel E. Austin1; Eric T. Sevy1; 1Brigham Young University, Provo, UT

TP 263
A Proton-Transfer-Reaction – Mass Spectrometry (PTR-MS) Setup with Real-Time Response for Low-Volatile Compounds; Alfons Jordan1; Felix Piel1, 2; Markus Müller1; Jenny Skytte af Sättra2; Klaus Winkler1; Tobias Reinecke1; Christian Lindinger1; Armin Wisthaler2; Lukas Märk1; Philipp Sulzer1; 1IONICON Analytik GmbH., Innsbruck, Austria; 2Department of Chemistry, University of Oslo, Oslo, Norway

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Gas Chromatography-Atmospheric Flow Tube-Mass Spectrometry (GC-AFT-MS) Analysis of Post-Detonation Explosive Residues; Kelsey A. Morrison1; Elizabeth H. Denis1; Robert G. Ewing1; 1Pacific Northwest National Laboratory, Richland, WA

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Enhanced Ionization and Facile Selection of Ions at Atmospheric-pressure by Perturbation-induced Pulsing of nano-ESI Coupled to a Single Ion Gate; William P. McMahan1; Kaveh Jorabchi1; 1Georgetown University, Washington, DC

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Experimental Investigation of Charged Nanodroplets in MS Transfer Stages originating from ESI plumes; Florian Stappert1; Clara Markert1; Marco Thinius1; Walter Wissdorf1; Hendrik Kersten1; Thorsten Benter1; 1University of Wuppertal, Wuppertal, Germany
TP 267 An Integrated Electrocatalytic nESI-MS Reaction Platform for In-situ Oxidation of C=C and C=O Bonds; Kavyasree Chintalapudi; The Ohio State University, Columbus

TP 268 Integrated Simulation of Rarefied Gas Dynamics and Ion Transport with a DSMC Method; Robin Hillen; Walter Wissdorf; Hendrik Kersten; Thorsten Benter; 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); Christian Gorgens; Katherine Walker; Cornelia Boesser; Neloni Wijeratne; Claudia Martins; Sven Guddat; Mario Thevis; Institute of Biochemistry, German Sport University Cologne, Cologne, Germany; Thermo Fisher Scientific, San Jose, CA; European Monitoring Center for Emerging Doping Agents (EuMoCEDA), Cologne/Bonn, Germany

TP 270 A Channel Electron Multiplier Based Ionization Source; Ely Driscoll; Stephen Ritzau; University of Connecticut, Storrs, CT; Photons USA, Inc., Sturbridge, MA

TP 271 Non-intrusive Tracking of Drugs of Abuse on Mail/Packaging Using Open Port Interface-Mass Spectrometry; Haidy Metwally; Prashant Agrawal; Rachael Smith; Chang Chang Liu; Yves Leblanc; Thomas R. Covey; Richard Oleschuk; Queen's University, Kingston, ON; SCIEX, Concord, Ontario

TP 272 Acoustic Droplet Ejection from Phase-Separated Liquid Ex extractions for High-Throughput Mass Spectrometry; Lucien Ghislain; Chang Liu; Eric Hall; Thomas R Covey; Xiujuan Wen; Kiersten Tovar; Sammy S Datwani; David G Mclaren; Beckman Coulter Life Sciences, San Jose, CA; SCIEX, Concord, Ontario; Merck & Co., Kenilworth, NJ

TP 273 Investigation of a fast and versatile analysis platform for screening and quantitation of explosives; Markus Weber; Jan-Christoph Wolf; Mario F. Mirabelii; TU Munich, Munich, Germany; Plasmion GmbH, Augsburg, Germany; CTC Analytics AG, Zurich, Switzerland

TP 274 Mechanism of Superoxide Adduct Formation in LDTD Ion Source Used in Quantitation; Pierre Picard; Francis Briere; Sylvain Letarte; Jean Lacoursiere; Serge Auger; Phytonix Technologies, Inc., Quebec, QC; Universite Laval, Quebec, Quebec

TP 275 Fluid Dynamic and Operational Considerations for an Acoustic Ejection Mass Spectrometry (AEFS) System for High Throughput Analysis; Chang Liu; Peter Kovarik; Thomas R Covey; SCIEX, Concord, ON

TP 276 Design and Evaluation of a Tethered, Handheld Sampling Probe for Liquid Extraction-Mass Spectrometry Analysis; Courtney Walton; John F. Cahill; Vilmos Kertesz; 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; Anthony Debastiani; Sandra N Majuta; Chong Li; Peng Li; Stephen J Valentine; West Virginia University, Morgantown

TP 278 Simulations of Collision Induced Evaporation Processes of Nanodroplets in MS Inlet Stages; Clara Markert; Walter Wissdorf; Hendrik Kersten; University of Wuppertal, Wuppertal, Germany

TP 279 Vibrating Sharp-edge Spray Ionization (VSSI) for Direct Analysis of Surface Samples using Mass Spectrometry; Nandhini Ranganathan; Austin M. Lozier; Michael C. Rawson; Matthew B. Johnson; Stephen J. Valentine; Peng Li; West Virginia University, Morgantown, WV

TP 280 Increasing the Resolution of Ion Mobility Separations with Broadly Applicable Ion/Ion Reagents; Ritu Chaturvedi; Ian Webb; Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN

TP 281 A Modular Machine Learning-Based, Multi-Chemical Class CCS Prediction Pipeline; Valentin Ianchis; Marisa Gioioso; Joanne Ballantyne; Johannes P.C. Vissers; Waters Corporation, Brasov, Romania; Waters Corporation, Milford, MA; Waters Corporation, Wilsom, United Kingdom

TP 282 Concurrent Ion Accumulation and Ion Mobility Spectrometry for Increased Ion Utilization; Ailin Li; Gabe Nagy; Isaac K. Attah; Christopher R. Conant; Adam L. Hollerbach; Richard D. Smith; Yehia M. Ibrahim; Sandiya V. B. Garimella; Pacific Northwest National Laboratory, Richland, WA

TP 283 A Fast Scanning Portable Differential Mobility Analyzer Incorporating a CTIA Detector; Kent Gillig; Da-Shung Su; Chung-Hsuan Chen; Academia Sinica, Taipei, Taiwan

TP 284 Towards automation of Collision Induced Unfolding experiments through online Size Exclusion Chromatography coupled to native Mass Spectrometry; Evolène Deslignière; Anthony Etkirch; Thomas Botanowski; Oscar Hernandez-Alba; Alain Beck; Sarah Cianferrari; Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; IRPF, Centre d’Immunologie Pierre Fabre, St-Julien en Genevois, France
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TP 285  Development of a high resolution Ion Mobility method and its application in prostate cancer metabolism; Sumankalai Ramachandran1; Minas Sakellakis2; Christopher Logothetis1, 3; Mark Titus1; 1MD Anderson Cancer Center, Houston, TX; 2Metropolitan Hospital, Neo Faliro, Greece; 3University of Athens, Athens, Greece

TP 286  Practical High Resolution Ion Mobility Mass Spectrometry Analyses with Structures for Lossless Ion Manipulations; John Daniel DeBord1; Kelly L. Wormwood Moser1; Jim Arndt1; Nathan Roehr1; Liulin Deng1; Gordon Anderson2; 1MOBILion Systems Inc., Chadds Ford, PA; 2GAA Custom Electronics, LLC, Richland, Washington

TP 287  A Prototype SLIM-based Ion Mobility Instrument for High Resolving Power Separations Integrated with MS; Jody C. May1; Katrina L. Leaprot1; Bailey S. Rose1; Kelly L. Wormwood Moser1; Daniel Dubord2; John A. McLean1; 1Vanderbilt University, Nashville, TN; 2MOBILion Systems, Inc., Chadds Ford, PA

TP 288  Characteristics analysis of modified oligonucleotides by ion mobility-mass spectrometry (IM-MS); Shogo Omuro1; Takao Yamaguchi1; Taiji Kawase1; Maki Terasak1; Kenji Hirose1; Satoshi Obika3; 1Graduate School of Pharmaceutical Sciences, Osaka University, 1-6 Yamadaoka, Suita, Japan; 2Nihon Waters KK, Kitashinagawa, Japan; 3Nihon Waters KK, Kitashinagawa, Japan

TP 289  Probing Protein Structural and Conformational Heterogeneity using Multiplexed Ion Mobility, High Resolution Mass Analysis, and Ultraviolet Photodissociation; James Sanders1; Jamie P. Butalewicz1; Sarah N. Sipe2; Virginia K. James2; Brian H Clowers3; Jennifer S. Brodbelt2; 1University of Texas, Austin, Austin, TX; 2University of Texas Austin, Austin, TX; 3Washington State University, Pullman, WA

TP 290  Flowing Atmospheric-Pressure Afterglow Drift Tube Ion Mobility Spectrometry; Mohsen Latif1; Gerardo Gamez2; 1Texas Tech University, Lubbock, TX

TP 291  Implementation and evaluation of electron capture dissociation (ECD) on a cyclic IMS enabled mass spectrometer; Joseph S. Beckman1, 2; Valery G. Voinov3; Darren Hewitt1; Jason Wildgoose1; Jonathan P. Williams4; Jeffrey M. Brown2; James I Langridge3; Dale A. Cooper-Shepherd4; 1Oregon State University, Corvallis, OR; 2e-MStion, Inc. Corvallis, OR; 3Waters Corporation, Wilmslow, United Kingdom; 4Waters Corporation, Wilmslow, United Kingdom; 5e-MStion Inc., Corvallis, Oregon

TP 292  Breaking Down Structural Diversity for Comprehensive Collision Cross Section Prediction Using Machine Learning; Dylan H Ross1; Jang Ho Cho1; Libin Xu1; 1Department of Medicinal Chemistry, Washington University, Seattle, WA

TP 293  The Effect of Solution Conditions on the Collisional Cross Section of GroEL; Joanna K Denton1; Jacob W. McCabe1; Christopher S. Mallis1; John M. Gordon1; David H. Russell2; 1Texas A&M University, College Station, TX

TP 294  Multiplexed Separations for Enhanced Duty Cycle Using Structures for Lossless Ion Manipulations; Brian H. Clowers1; Elvin Cabrera1; Liulin Deng1; Kelly Moser2; Gregory Van Aken2; John Daniel DeBord2; 1Washington State University, Pullman, WA; 2MOBILion 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 Deng1; Nathan Roehr1; Gordon Anderson2; Daniel Debord1; 1MOBILion Systems Inc., Chadds Ford, PA; 2GAA Custom Electronics, LLC, Richland, Washington

TP 296  Cyclic ion mobility spectrometry coupled to high-resolution mass spectrometry — Prospects for complex mixture analysis; Christopher Paul Rügjer1; 2; Johann Le Maitre2; 3; Martin Palmer4; Eleanor Riches4; Carlos Afonso2; 3; Pierre Giusti2; 3; 1University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; 2International Joint Laboratory - IC2MC: Complex Matrices Molecular Characterization, Harfleur, France; 3Total Refining and Chemicals, Harfleur, France; 4Waters Corporation, Wilmslow, United Kingdom; 5University of Rouen-Normandy, Mont-Saint-Aignan, France

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TP 297  Correlating Gas-Phase Unfolded Conformations To In-Solution Structures Using Single-and Multi-Stage Ion-Mobility and Gas-Phase Simulations; Charles Eldred1; Tristan Cragnolin1; 2; Aisha Ben-Younis1; Junjie Zou3; Daniel Raleigh1, 3; Konstantinos Thalassinos1; 1University College London, London, United Kingdom; 2Birckbeck, London, United Kingdom; 3Stonybrook University, Stonybrook, NY

TP 298  Peptide structure confirmation based on molecular weight and collision cross section obtained with; Stuart Pengelley1; Thomas Schmitz2; Diana Imhof2; Detlev Suckau1; 1Bruker Daltonics, Bremen, Germany; 2University 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. Leaprot1; Bailey S. Rose1; Jody C. May1; Kelly L. Wormwood Moser2; John A. McLean1; 1Vanderbilt University, Nashville, TN; 2MOBILion 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 Grammel1; Max Kramer1; Sebastian Kandzia1; Romano Hebele2; Christian Albers3; Alvo Tech Hannover, Hanover, Germany; 3Bruker 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 May1; Shawn T. Phillips1; Emanuel Zlibut2; Martin Palmer2; James I Langridge3; John A. McLean1; 1Vanderbilt University, Nashville, TN; 2Waters Corporation, Wilmslow, United Kingdom

TP 302  Evaluation of Computational Strategies to Interpret Ion Mobility Measurements for Chemically-Diverse Analytes; Emanuel Zlibut2; Berkley Ellis3; Jody C. May1; John A. McLean1; 1Vanderbilt 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 Mehboob1; James Scrivens1; Jackie A Mosely1; David E Portwood2; Pablo Navarro2; Martin Palmer2; Jakub Ujma2; Kevin Giles2; 1Teesside University, Middlesbrough, United Kingdom; 2University College London, London, 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 Kit1; Ian K Webb1; 1Department 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 Stuchfield1; Jack Roberts1; Perdita E Barran1; 1The University of Manchester, Manchester, United Kingdom

TP 307  Structural characterization of polyurethane oligomers and synthetic homopolymers by ion mobility-mass spectrometry; Kevin M Buck1; Rachel A. Harris1; Jody C. May1; Ian D. Tomlinson1; John A. McLean1; David M. Hercules1; 1Vanderbilt 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 Chai1; Tyler C Copley1; Fanny C. Liu1; Christian Bleiholder1; Florida State University, Tallahassee, FL

TP 310  Two-Dimensional Differential/Linear Ion Mobility Separations of Protein Conformations; Jacob Porter1; Alexandre Shvartsburg; Francisco A. Fernandez-Lima1; 1Florida International University, Miami, FL; 2Wichita State University, Wichita, KS

TP 311  Conformational Dynamics of Chaperonin Complexes using nESI-CIA-TIMS-MS; Kevin Jeanne Dit Fouque1; Prem P. Chapagain1; Francisco Fernandez-Lima1; 1Florida 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. Attygalle1; Zhaoyu Zheng1; 1Stevens Institute of Technology, Hoboken, NJ; 2Stevens Institute of Technology, Hoboken, NJ

TP 313  Lanthipeptide Topoisomerase Screening Based on TIMS-MS/MS; Kevin Jeanne Dit Fouque1; Tung T. Le2; Julian D. Hegemann3; Wilfred Van Der Donk2; Francisco Fernandez-Lima1; 1Florida International University, Miami, FL; 2University of Illinois at Urbana-Champaign, Urbana, IL; 3Technische 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 Raab1; David A. Hales2; Wen Liu3; Yang Liu4; Arthur Laganowsky1; David H. Russell1; David E. Clemmer1; 1Indiana University, Bloomington, IN; 2Hendrix College, Conway, AR; 3Texas A&M University, College Station, TX

TP 315  The Apparent Density: a critical ion property to consider for ion mobility mass spectrometry analysis; Christopher Kune1; Raphaël La Rocca1; Andréa Mc Cann1; Jean R. N. Haler1; Sophie Rappe1; Janina Oetjen1; Gauthier Eppe1; Johann Far1; Edwin De Pauw1; 1University of Liege, Liège, Belgium; 2Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; 3Bruker 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 Wilson1; Samuel W Maddox1; Aurora Burkus-Matesevac1; Christopher D. Chouinard1; 1Florida Institute of Technology, Melbourne, FL

TP 317  Variable-Temperature Ion Mobility: A ‘Cool’ Study of IgG Antibody Conformations; Perdita E Barran1; Emma Norgate1; 1University 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-Younis1; Charles Eldrid1; Alexander Zhyvoloup1; Hannah M. Britt1; Daniel Raleigh1; 1; Konstantinos Thalassinos1; 1University College London, London, United Kingdom; 2Stony Brook University, Stony Brook, NY
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**TP 319** Collisional-Induced Unfolding and Dissociation of Streptavidin in Tandem-Trapped Ion Mobility Spectrometry/Mass Spectrometry (Tandem-TIMS/MS); Wesley Ferguson1; Valentina Rangel1; Fanny C Liu1; Christian Bleiholder1; 1Florida 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 Rangel1; Fanny C Liu1; Christian Bleiholder1; 1Florida State University, Tallahassee, FL

**TP 321** A new ion mobility tandem mass spectrometer for isomer-specific fragmentation and cryogenic IR spectroscopy of glycans; Lei Yue1; Robert P Pellegrinelli1; Eduardo Carrascosa1; Stephan Warnke1; Ahmed Ben Falah1; Thomas R. Rizzo1; 1EPFL/LCPM, Lausanne, Switzerland

**TP 322** Analysis of Synthesized Polyethylene Glycol-Based Polyurethane Oligomers Using Ion Mobility-Mass Spectrometry; Rachel Harris1; Kevin M Buck1; Sahil Soni1; Jaqueline A. Picache2; Ian D. Tomlinson1; Emanuel Zilbut1; Berkley M. Ellis1; Jody C. May1; John A. McLean1; David M. Hercules1; 1Vanderbilt Univeristy, Nashville, Tennessee

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**TP 323** Comprehensive Degradant Identification and Management of Analytical Data in Drug Product Development; Joe Dimartino1; Andrew A. Anderson1; Sanjivanjit K. Bhal1; 1ACD/Labs, Toronto, ON

**TP 324** Development of an analytical reversed phase column for characterization of intact antibodies using wide pore monolithic silica; Shigenori Ota1; Yuko Yui1; Shota Miyazaki2; Chiaki Aoyama1; Ken Miyashita1; Manami Takeda1; Shunta Futagami1; Tsutomu Sato1; 1GL Sciences Inc., Saitama, Japan; 2GL Sciences Inc., Tokyo, Japan

**TP 325** A Novel Mass Spectrometry Peak Tracking Tool for Analytical Quality by Design Method Development; Fadi L Alkhateeb1; Paul Rainville1; Nathan Anderson1; 1Waters Corporation, Milford, MA

**TP 326** Peptide retention time prediction for TMT-labeled peptides in 2D LC-MS/MS experiments (HLIC, SCX, high pH RP/low pH RP); Benilde Mizerow1; Carina Villacres2; Victor Spicer2; Rosa Viner3; Julian Saba3; Bhavinkumar Patel Patel4; Sergei Snovida5; Penny Jensen6; Andreas Huhmer7; Oleg Krokhin1,8; 1University of Manitoba/Department of Chemistry, Winnipeg, Manitoba; 2Manitoba Centre for Proteomics and Systems Biology / Department of Internal Medicine, University of Manitoba, Winnipeg, Canada, Winnipeg, MB; 3Thermo Fisher Scientific, Scottsdale, AZ; 4Thermo Fisher Scientific, Mississauga, Ontario; 5Thermo Fisher Scientific, Rockford, IL

**TP 327** High Throughput Mass Deconvolution Software to Identify and Quantitate Intended and Mispaired Heteroglycopic Antibody Molecules; John Robinson1; Hannah B. Catterall1; John O. Hui1; Iain D. G. Campuzano1; 1Amgen 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 Qin1; Rufeng Li1; Hong Shao1; Qiu Lin2; Jennifer Copeland2; Martin Brisbin2; Hal Barnett2; Huanan Cai2; Stan Stearns2; Chengzhi Cai1; 1University of Houston, Houston, TX; 2VICI 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 Yin1; Zheng-Jiang Zhu2; 1Interdisciplinary Research Center on Biology and Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China; 2Interdisciplinary Research Center of 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 Osipenko1; Inga Bashkirova1; Sergey Sosnin1; Yury Kostyukevich1; Eugene (evgeny) Nikolaev1; 1Skolkovo institute of science and technology, Moscow Region, Russian Federation

**TP 331** Quantitative Amino Acid analysis in Cell Culture Media Using SWATH® Acquisition; Zuzana Demianova1; Jeff Layne2; Brian Rivera2; Chad Eichman3; Lei Xiong4; 1Sciex, Brea, CA; 2Phenomenex, Torrance, CA; 3SCIEX, Redwood Shores, California 1201

**TP 332** Improved Performance of Modern MS-Compatible Reversed-Phase/Anion-Exchange Mixed-Mode HPLC Columns; Thomas H. Walter1; Bonnie A. Alden1; Melvin Blaze1; Cheryl Boiselle1; Donna Osterman1; Amit V. Patel1; Mathew Delano1; Nicole Lawrence1; Jessica Field1; Moon Chul Jung1; 1Waters Corporation, Milford, MA

**TP 333** Expression proteotomics of Clostridium septicum using LC-MS/MS analysis Dominik B, Mendes M,A Temple University, Philadelphia, Dempster MS Lab, San Paulo Brazil; Barbara Dominiak; 1Temple 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 Zhou1; John Ma1; Silverio Iacono2; Sharon Tong1; 1WuXi AppTec, Cranbury, NJ; 2Tomtec Inc, Hamden, CT
Carboxylate modified magnetic bead (CMMB)-based peptide fractionation enables rapid and robust off-line peptide mixture simplification in bottom-up proteomics; Weixian Deng¹; Jihui Sha¹; James A. Wohlschlegel¹; ¹UCLA, Los Angeles, CA

Bioanalytical challenges with BioChaperone® BC structures to quantify parent and truncated metabolite in rat, dog, rabbit and human plasmas; Gregoire Haricha²; Jordan Goncalves²; Mouhssin Oufir²; Remi Thouvinon³; Peran Terrier³; Segolene Laage³; Yann Courbebaisse³; Fabrice Viviani³; ¹Oncodesign, Villebon-Sur-Yvette, France; ²ADOcia, LYON, France

Accomplishing all new challenges for the β-glucuronidases; Camila Berens¹; Jack Andrews¹; Jose Luis Callejas¹; Nicholas Chestara²; ¹Kurabiotech, Puerto Varas, Chile; ²DPX Technologies, Columbia, South Carolina

Improved peptide recovery during proteolytic digestion of low-level protein samples by a simple modification to the FASP approach; Jennifer J Hill¹; Tammy-Lynn Tremblay¹; ¹National Research Council Canada, Ottawa, ON

Digestion efficiency in cartridge and bead-based workflows for bottom-up proteomics; Jessica L. Nickerson¹; Alan A. Doucette¹; ¹Dalhousie University, Halifax, NS

Micro extraction and LC/MS/MS analysis of multi-class pharmaceutical compounds in human plasma using Solid Phase Extraction Tips; Jama Shafoe³; Keynoush Naraghi³; Corentin Germain³; Sami Bayoudh³; Raphael Durand³; Michel Arocoarena³; ¹AFFINISEP, Petit Couronne, France

Simplified Sample Preparation for Drugs of Abuse Extraction from Urine Samples Prior to LC-MS/MS Analysis; Geoff Davies¹; Lee Williams¹; Rhys Jones¹; Kati-Jo Teehan¹; Adam Senior¹; Alan Edgington¹; Helen Loder¹; ¹Biotage GB Limited, Cardiff, United Kingdom

Optimized Sample Preparation and Off-Line High pH Reversed-Phase Fractionation for TMTpro-labeled Proteomics Samples; Sergei Snovida¹; Amarjeet Flora¹; Ryan Bomgarden¹; John C Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL

Ultra-Fast Analysis of Nitrosamines Using SPE-QQQ; Kevin Truempi¹; Kevin Mccann¹; ¹Agilent Technologies, Santa Clara, CA

Less is more: Avoiding artificial modifications in proteomic sample preparation for pharmaceutical and clinical applications; Katrin Hartinger¹; Sebastian H. Johansson¹; Nils A. Kukl¹; Katharina Scheck¹; Fabian Hosp¹; ¹PreOmines GmbH, München, Germany

Fully Automated Sample Preparation Platform for Peptide Mapping and Protein Identification by Mass Spectrometry; Jia Tang¹; Yi Zeng¹; Billy Newton¹; Guanghui Han¹; Chri Suh²; Rachel Keating²; Lee Hoang²; ¹BGI Americas, San Jose, CA; ²PhyNexus now part of Biotage, San Jose, CA

Low-cost nanoliter pipetting platforms for automated preparation of nanoscale and single-cell proteomic samples; Yiran Liang¹; Enoch A. W. Councill¹; Hayden Acor¹; Nathaniel B. Axtel¹; Adam L. Aposhian¹; Thy Truong¹; Yongzheng Cong²; Ying Zhu²; Richard H. Carson²; Ryan T. Kelly¹; ¹Brigham Young University, Provo, UT; ²Pacific Northwest National Laboratory, Richland, WA

Novel MS compatible surfactant for high temperature protein sample preparation: maximizing protein recovery and digestion efficiency; Valerie T Ressler¹; Sergei Saveliev¹; Wenhiu Zhou¹; Joel Walker¹; Jean Osterman¹; Mike Rosenblatt¹; Poncho Meisenheimer¹; Marjeta Urh¹; ¹Promega Corporation, Madison, WI

Unsaturation Elements and other Modifications of Phospholipids in Bacteria: New Insight from UVPD Mass Spectrometry; Molly S. Blevins¹; Virginia K. James¹; Carmen M. Herrera¹; Alexandria B. Purcell¹; M. Stephen Trent¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²University of Georgia, Athens, GA

Double bond localization in unsaturated FAME by CI-MS/MS collisional dissociation of acetonitrile adduct [M+40]+; Zhen Wang¹; Dong Hao Wang¹; J. Thomas Brenna²; ¹University of Texas at Austin, Austin, TX; ²Cornell University, Ithaca, NY

A Simple MALDI/TOF Technique Reveals the Acyl Double-Bond Positions on the Fatty Acyl Coenzyme A Esters; Hay-Yan J Wang¹; Fong-Fu Hsu²; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Washington University in St. Louis, Saint Louis, MO

Integrating Qual/Quan Workflows for Combined Structure Characterization and Quantitation of Vinyl Ether Phosphatidylethanolamine; Yulemni Morei¹; Chinmoy Sarkar¹; Maureen A Kane¹; Marta Lipinski¹; Jace W.
TP 352 4D-Lipidomics investigation in search of the fountain of youth; Aiko Barsch1; Sven W. Meyer1; Ulrike Schweiger-Hufnagel1; Philippe Schmitt-Kopplin2, 3; Michael Witting2, 3; 1Bruker Daltonics, Bremen, Germany; 2Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, Neuherberg, Germany; 3Chair 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 Macias1; Clara L. Feider1; Livia S. Eberlin1; Jennifer S. Brodbelt1; 1University of Texas - Austin, Austin, TX

TP 354 Comprehensive analysis of lamincin biosurfactants by means of LC-MS; Karen Scholz1; Till Tiso2; Heiko Hayen3; 1University of Münster - Institute of Inorganic and Analytical Chemistry, Münster, Germany; 2RWTH Aachen University, iAMB - Institute of Applied Microbiology, ABBI – Aachen Biology and Biotechnology, Aachen, Germany; 3Institute 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 Seyer1; Benoit Colsch1; Annelaure Damont1; Sylvain Dechaumet1; Christophe Junot1; François Fenaille1; Jean-Claude Tabet1; 1MedDay Pharmaceuticals, Paris, France; 2Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), Gif sur Yvette, France; 3UPMC-CEA, Morangis, France

TP 356 Analysis of bacterial lipids using 13C-TrEnDi derivatization and ultraviolet photodissociation mass spectrometry; Molly S. Blevins1; Samuel W Shields1, 2; Jeffrey C Smith2; Jennifer S Brodbelt1; 1University of Texas at Austin, Austin, TX; 2Carleton University, Ottawa, ON

TP 358 Deploying ozone-induced dissociation for targeted and untargeted lipidomic workflows reveals hidden isomeric complexity; Berwynk Poad1; Adam M King2; Christopher R. Douglas3; Reuben S. E. Young1; Martin Green1; Lee A Gethings2; Todd W Mitchell1; Stephen J. Blanksby1; 1Queensland University of Technology, Brisbane, Australia; 2Waters Corporation, Wilmslow, United Kingdom; 3University 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 Gachotte1; Yelena Adelfinskaya1; Jeff Gilbert2; Ralf Tautenhahn1; Yasuto Yokoi1; 1Corteva, Indianapolis, IN; 2University of Maryland, School of Pharmacy, Baltimore, MD; 3Bruker Daltonics, Bremen, Germany

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 Duchoslav1; Pavel Ryumin2; Jason Causon2; Takashi Baba1; 1SCIEX, Concord, ON; 2SCIEX, Concord, Ontario

TP 361 Fatty Acid Structural Elucidation by Pairing the Paternó–Büchi Reaction with Gas-phase Ion/Ion Chemistry using Tris-Phenanthroline Earth Metal Reagents; De’shovan M Shenault1; Elissia T. Franklin1; Scott A. Mcluckey1; 1Purdue University, Lafayette, IN

TP 362 From Static Electricity to Structure: Triboelectric Nanogenerators for Unsaturated Lipid Double Bond Pinpointing; Marcos Bouza Areces1; Yafeng Li1; Changsheng Wu1; Hengyu Guo1; Zhong L. Wang1; 2Mitsui Knowledge Industry Co., Ltd., Tokyo, Japan; 1Georgia Institute of Technology, Atlanta, GA; 2Beijing 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 Chemistry using Tris-Phenanthroline Earth Metal Reagents; Elissia T. Franklin1; De’shovan M Shenault1; Scott A. Mcluckey1; 1Purdue 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 Ross1; Jang Ho Cho1; Rutan Zhang1; Emily L Pruitt2; Libin Xu1; 1Department of Medicinal Chemistry, University of Washington, Seattle, WA; 2Department 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 Khorani1; Jeffrey Morre1; Armando Alcazar Magana1; Claudia Susanne Maier1; 1Department of Chemistry, Oregon State University, Corvallis, Oregon 97331

TP 366 Construction of novel lipidomics workflow using TMT derivatization and LipidSearch5.0; Yasuto Yokoi1; Suzumi M Tokuoka2; Megumi Ishibashi2; Yoshiya Oda2; 1Mitsui Knowledge Industry Co., Ltd., Tokyo, Japan; 2The University of Tokyo, Graduate School of Medicine, Lipidomics Laboratory, Tokyo, Japan; 3Thermo Fisher Scientific, Kanagawa, Japan, Yokohama, Japan

TP 367 On-Demand Electrochemical Strategies in Mass Spectrometry for Lipid Analysis; Shuli Tang1; Heyong Cheng1; Xin Yan1; 1Texas A&M University, College Station, TX; 2Hangzhou Normal University, Hangzhou, China
**ASMS 2020 Reboot**

**TP 371**

**Calibrating nonlinear ESI responses using quality control samples to overcome quantitative errors in mass spectrometry-based metabolomics**

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TP 382  Characterization of Gut-Brain Axis Communication of Tryptophan Metabolites Using UHPLC-HRMS; Richard C Dilworth1; Vanessa Y. Rubio2; Gary P Wang3; Richard A Yost4; Timothy J Garrett5; 1University of Florida, Gainesville, FL; 2University 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 Baumann1; Nic D Leipzig1; Leah P Shriver1; 1University of Akron, Akron, OH

TP 385  On the Origin of Protons in Electrospray Ionization; Yixin Zhu1; Kai Tang2; 1Zhejiang Haochuang Biotech Co. Ltd., Hangzhou, China

TP 386  Merging untargeted and targeted analysis of the lipidome, metabolome, and exposome; Tomas Cajka1; Jiri Hricko2; Michaela Novakova1; Michaela Paucova1; Ondrej Kuda1; 1Institute of Physiology CAS, Prague, Czech Republic

TP 387  Evaluation of LC-MS mobile-phase modifiers for metabolomic and lipidomic profiling; Jiri Hricko1; Tomas Cajka1; Michaela Paucova1; Michaela Novakova1; 1Institute of Physiology CAS, Prague, Czech Republic

TP 388  Compound identification strategies in metabolomics: What if MS/MS is not enough?; Charles R Evans1; Brady G Anderson1; Alla Karnovsky1; Hani Habra1; Maureen T Kachman1; Alexander B Raskind1; 1University 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 Zhang1; Anthony Andrea2; Costas Lyssiotis3; 1University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan; 2University of Michigan School of Medicine, Rogel Cancer Center, Ann Arbor, Michigan; 3University 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 Guan1; 2; Michael R. Armbruster1; 3; James L. Edwards1; Benjamin J Bythell1; 2; 1Ohio University, Athens, OH; 2University of Missouri, St. Louis, St. Louis, MO; 3Saint 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-Manso1; Xinjiang Yan1; Kelly H. Telu1; Yuri A. Mirokhin1; Yuxue Liang1; Stephen E. Stein1; 1NIST, Gaithersburg, MD

TP 393  Untargeted Screening in a Case Control Study Using Apples as a Matrix; Erica L Bakota1; Robert A Levine1; 1U.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. Kramer1; 2; Feng Qiu1; 2; 3; Barbara W Sumner1; 2; 2; Sean M. Colby1; Ryan S. Renslow1; Thomas O. Metz1; Lloyd W. Sumner1; 2, 3; 1Department of Biochemistry, University of Missouri, Columbia, MO; 2Department of Missouri Metabolomics Center, Columbia, Missouri; 3International Flavor and Fragrance, Union Beach, NJ; 4Pacific Northwest National Lab, Richland, WA

TP 395  Metabolite Profiling of Centella asiatica L. Leaves using Ultrahigh Resolution Fourier Transform Ion Cyclotron Mass Spectrometry; Syful Islam1; 2; Sungwhan Kim1; 3; 1Department of Chemistry, Kyungpook National University, Daegu, South Korea; 2Department of Environment, Munshiganj District Office, Munshiganj, Bangladesh; 3Green-Nano materials Research Center, Daegu, South Korea

TP 396  Unravelling via Mass Spectrometry the L-Argininosuccinic acid cyclization in biological samples; Ana Gradillas1; Manicruz Mamani-Huancaya1; Angeles Lopez-Gonzalez1; Coral Barbosa1; 1CEMIBIO, 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 Gunner1; Nathan Lawler1; Berin Boughton1; Melvin C.L. Gay2; Samantha Lodge1; 2; Christopher Thompson4; Elaine Holmes1; 5; Jeremy Nicholson1; 5; 1Australian National Phenome Centre, Murdoch University, Murdoch, Australia; 2Bruker Pty Ltd, Preston, Australia; 3Health Futures Institute, Murdoch University, Murdoch, Australia; 4Bruker Daltonics, Billerica, MA; 5Research and Innovation Office, Murdoch University, Murdoch, Australia

TP 398  MetFID: Metabolite Annotation Using Artificial Neural Network; Ziling Fan1; Amber Alley2; Kian Ghaffari1; Habtom Ressom1; 1Georgetown University, Washington, DC

TP 399  Identifying plant natural products in the food we eat by untargeted metabolomics; Arpana Vaniya1; Ying Y. Choy1; Alberto Valdés1; Sajjan Singh Mehta1; John de la Parra2; Carol D. Stroble1; Tong Shen3; Luis M. Valdiviez1; Michael Sebek3; Rebekah Carlson4; Caleb Harper5; 1Oliver Fiehn1; 2West Coast Metabolomics Center, UC Davis, Davis, CA; 3Harvard University Herbaria, Cambridge, MA; 4Pacific Northwest National Lab, Richland, WA; 5Research and Innovation Office, Murdoch University, Murdoch, Australia
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**Microorganisms and the Microbiome II**

**TP 400**
Metabos: A Suite of Tools for Metabolite Annotation; Habtom W Ressom1; Linge Yan1; Mohammad R Nezami-Ranjbar1; OmicsCraft, Washington, District of Columbia

**TP 401**
Untargeted vs amine targeted metabolomics of MRSA to identify antibiotic agent biomarkers; Amar Deep Sharma1; Nitish R. Mishra1; William G. Gutheil1; University of Missouri-Kansas City, Kansas City, MO

**TP 402**
Paired mass distance dependent analysis (PMDDA) for robust untargeted compound identification; Miao Yu1; Lauren Petrick1; Georgia Dolios1; Icahn School of Medicine at Mount Sinai, New York, NY

**TP 403**
Analysis of Penillium sclerotiorum specialized metabolome by molecular networking; Teo Hebra1; Veronique Eparvier1; David Touboul1; CNRS-ICSN, Institut de Chimie des Substances Naturelles, UPR 2301, Université Paris Saclay, Orsay, France

**TP 404**
Robust Accurate Identification and Biomass Estimates of Microorganisms via Tandem Mass Spectrometry; Gelio Alves1; Yi-Kuo Yu1; National Center for Biotechnology Information, NLM, Bethesda, MD

**TP 405**
Metabolomics analysis of colorectal cancer-associated anaerobic bacteria co-cultured with tumor spheroids; Thomas P Wyche1; Stephen H Kasper1; Carolina Morelli-Perez1; Linda A Lieberman1; Erik C Hett1; Theodore R Sana1; Exploratory Science Center, Merck & Co., Inc., Cambridge, MA

**TP 406**
Identifying heat stress correlated metabolites in reef building corals; Eric N Chiles1; Amanda Williams2; Debashish Bhattacharya2; Xiaoyang Su3, 4; Metabolomics Shared Resource, Rutgers University, New Brunswick, NJ; Department of Biochemistry and Microbiology, Rutgers University, New Brunswick, NJ; 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; David R Goodlett1; Francesca Gardener2; Hyojik Yang3; Sung Hwan Yoon4; Tao Liang5; Courtney Chandler2; Robert K Ernst1; Matthew Sorensen6; Erik Nilsson7; University of Maryland, Baltimore, MD; International Centre for Cancer Vaccine Science, Gdansk, Poland; University of Maryland Baltimore, Baltimore, MD; NIH, Bethesda, Maryland; Pataigain, LLC, Baltimore, MD

**TP 408**
Bile Acid Profile and its Changes in Response to Cefoperazone Treatment in MR1 Deficient Mice; Jinchun Sun1; Zhijun Cao1; Ashley D. Smith2; Paul E. Carlson Jr3; Michael Coryell2; Huizhong Chen1; Richard Beger1; NCTR / USFDA, Jefferson, AR; CBER, Silver Spring, MD; CBER, Silver Spring, MS

**TP 409**
Complex Community Metabolite Interactions from the Cheese Rind-Derived Microbiome; Gordon T Luu1; Jessica Cleary1; Emily C Pierce2; Rachel J Dutton2; Laura M Sanchez1; University of Illinois at Chicago, Chicago, IL; UCSD, La Jolla, CA

**TP 410**
Optimization of protein extraction methods to study root-associated microbes with metaproteomics; Fernanda Salvato1; Clara Tang2; Omri Finkel1; Jeffery L. Dang3; Ben Niu4; Manuel Kleiner2; North Carolina State University, Raleigh, NC; North Carolina State University, Raleigh, NC; University of North Carolina at Chapel Hill, Chapel Hill, NC; 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; Sigmund J. Haideracher1; 2; Thomas D. Horvath1; 2; Kathleen M. Hoch1; 2; Melanie A. Engevik1; 2; Faith D. Ihekweazu1; 2; Anthony M. Haag1; 2; Baylor College of Medicine, Houston, TX; Texas Children’s Hospital - Microbiome Center, Houston, TX

**TP 412**
Extraction Development for Metabolomics Analysis of the Cystic Fibrosis Pulmonary Microbiome; Brent D Carrillo1; Vanessa Phelan1; CU Denver Anschutz Medical Campus, Aurora, CO

**TP 413**
Rapid differentiation of antibiotic-resistant Staphylococcus aureus using secondary electrospray ionization mass spectrometry; Jiangjiang (chris) Zhu; The Ohio State University, Columbus, OH

**TP 414**
Biosynthesis pathway of indole-3-acetic acid in Candida tropicalis; Masaru Miyagi1; Christopher L. Hager1; Thomas Mc Cormick1; Mahmoud A. Ghannoun1; Case Western Reserve University, Cleveland, OH

**TP 415**
Metaproteomic analysis of murine gut and nasopharyngeal microbiomes in response to infection; Joby Cole1; 2; Caroline Evans3; Mark Dickman1; The Florey Institute, Sheffield, United Kingdom; Department of Infection, Immunity & Cardiovascular Diseases, Sheffield, United Kingdom; Department of Chemical and Biological engineering, Sheffield, United Kingdom

**TP 416**
Mapping of bacterial metabolism with stable-isotope labeled tracers and HRAM-LC-MS; Thomas D Horvath1; 2; Qinglong Wu1; 2; Sigmund J. Haideracher1; 2; Kathleen M. Hoch1; 2; Tor C. Savidge1; 2; Anthony M. Haag1; 2; Baylor College of Medicine, Houston, TX; Texas Children’s Hospital - Microbiome Center, Houston, TX
LC-MS-MS Identification of Bacteriophage and Host Peptides after CsCl gradient isolation; Leslie Harden; Yen-Te Liao; Vivian C. H. Wu; USDA/WRRC, Albany, CA

Urinary protein protein and its effect on biofilm formation on urinary catheters by nonpathogenic and pathogenic bacteria; Rufeng Li; Guoting Qin; Yanxin Chen; Mengfan Wang; Christopher Thang; Chengzhi Cai; University of Houston, Houston, TX

Characterization of substrate specificity of Staphylococcus aureus secreted lipases using HILIC-ion mobility-mass spectrometry; Emily L Pruit; Tianwei Shen; Rutan Zhang; Dylan H Ross; Xi Chen; Francis Alonzo lii; Labin Xu; Matthew F. Bush; Department of Chemistry, University of Washington, Seattle, WA; Department of Medicinal Chemistry, University of Washington, Seattle, WA; Department of Microbiology and Immunology, Loyola University, Chicago, IL

In-depth structure characterization of lipopolysaccharide via integration of chromatography, ion mobility, and high-resolution tandem mass spectrometry; Cassandra E Nelson; Eugene Moskovets; Amanda Oglesby-Sherrouse; Jace W Jones; University of Maryland School of Pharmacy, Baltimore, MD; Mass Tech, Inc., Columbia, MD; University of Maryland, School of Pharmacy, Baltimore, MD

Mass spectrometry-based mapping of rabbit ocular surface proteome and microbiome; Guoting Qin; Chengzhi Cai; University of Houston, Houston, TX

Combined LC-MS and Microflow 1H NMR strategy for the identification of volume and mass-limited lipid isomers; Jiajun Lei; Matthew E. Merritt; Richard A Yost; University of Florida, Gainesville, FL

Capillary flow LC-MS using micro pillar array columns: combining nano flow sensitivity with analytical flow robustness and throughput; Geert Van Raemdonck; Jeff Op De Beeck; Paul Jacobs; Gert Desmet; PharmaFluidics, Zwijnaarde, Belgium; Vrije Universiteit Brussel, Brussels, Belgium

A new high-pressure station for the multiplexed packing of capillary columns; Johannes B Müller; Peter V Treit; Lisa C Schweizer; Philipp E Geyer; Matthias Mann; Max Planck Institute of Biochime, Martinsried, Germany; Max Planck Institute of Biochemistry, Martinsried, Germany; Max Planck Institute of Biochemistry, München, Germany; NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark

μRIPS - Microfluidic Refrigeration Induced Phase Separation for ESI-MS Analysis of Complex Biochemical Samples; Austin L. Culberson; Yury Desyaterik; Jean P Alarie; Glenn A Harris; Kenion H Blakeman; Ryan R Barton; J. Michael Ramsay; UNC Chapel Hill, Chapel Hill, NC; 908 Devices, Inc., Boston, MA; North Carolina State University, Raleigh, NC

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

Development of UPLC-MS Method for Global RNA Modification Analysis in SaccharomycesCerevisiaeRNAs; Qishan Lin; University at Albany, Albany, NY

A Whole New World: TEA and HFIP free LC-MS conditions for siRNA analysis to enable monitoring of small molecule impurities; Jennifer Lippens; Shawn Pope; Laura Blue; Tawnya Flick; Amgen, Thousand Oaks, CA

Liquid chromatography-based fractionation of eukaryotic transfer RNA for improved RNA modification mapping by LC-MS/MS; Gwenn G. Parungao; Scott Abernathy; Manasses Jora; Robert Ross; Balasubrahmanyam Addepalli; Patrick A. Limbach; University of Cincinnati, Cincinnati, OH

Pytheas: a platform for the identification, mapping and statistical analysis of RNA post-transcriptional modifications via LC-MS; Luigi D'ascenzo; Anna Popova; James R. Williamson; The Scripps Research Institute, La Jolla, CA

Evaluation of a new software tool for assisting with the siRNA metabolite identification by LC-MS; Babak Basiri; Wilfred Tang; Marshall Bern; Yong J Kil; Maria Basanta-Sanchez; Mei Han; Fang Xie; Brooke M. Rock; Amgen Inc., South San Francisco, CA; Protein Metrics, Cupertino, CA
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TP 433  A Scheduled LC-MS3Method for Assessing the Epitranscriptome; Gwendolyn Gonzalez1; Yuxing Cui1; Yinsheng Wang1; Pengcheng Wang1; 1University 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; Peter Rye1; Yanan Yang2; 1Agilent, Lexington, MA; 2Agilent Technologies, Santa Clara, CA

TP 435  “xNA Analyzer”: a novel computational tool for characterizing therapeutic oligonucleotides using liquid chromatography-tandem mass spectrometry data; Yuki Matsubara1; Yasuto Yasko1; Masami Koike2; Masato Taoka3; Yuko Nobe3; Hiroshi Nakayama2; 1Mitsui Knowledge Industry, Tokyo, Japan; 2RIKEN CSRS, Wako, Japan; 3Tokyo 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; Dennis Kraus1; Noah Post2; Shannon Hall3; Fumin Li1; 1PPD, Middleton, WI; 2Ionis Pharmaceuticals, Inc, Carlsbad, CA

TP 437  Understanding retention mechanisms of oligonucleotides during hydrophilic interaction liquid chromatography mass spectrometry; Scott Abernathy1; Peter A. Lobue1; Naman Dhingra1; Balasubrahmanyam Addepalli1; Patrick A. Limbach1; 1University of Cincinnati, Cincinnati, OH

TP 438  Detection of complex tRNA modifications by mass spectrometry using NucleicAcidSearchEngine; Samuel P Wein1; Byron Andrews2; Hendrik Weisser2; 1University of Tübingen, Tübingen, Germany; 2Storm Therapeutics, Cambridge, United Kingdom

TP 440  A MSMS auto-workflow for synthetic oligonucleotide sequence confirmation; Walter Wang; Alnylam, Cambridge, MA

TP 441  Deinococcus radiodurans Transfer RNA Modified Nucleosides are Minimally Impacted by UVA Radiation; Ruoxia Zhao1; Spencer Parrish1; Robert L. Ross1; Manasses Jora1; Balasubrahmanyam Addepalli1; Patrick A. Limbach1; 1University of Cincinnati, Cincinnati, OH

TP 442  Quantitative determination of PMOs and PPMOs in mouse and monkey tissues by UPLC-HRMS; John Chen1; Jianbo Zhang2; Ran An3; Jian Shi1; Chengjie Ji1; John Hadcock2; 1Novabioassays LLC, Woburn, MA; 2Sarepta Therapeutics, Cambridge, MA

TP 443  Climbing the oligonucleotide ladder toward rapid and wide-ranging oligonucleotide analysis using benchtop MALDI-MS; Dominique B Figueroa1; Vikki Johnson1; M. Nazim Boutaghou2; Jordan Frost1; 1Shimadzu Scientific Instruments, Inc, Carlsbad, CA; 2Shimadzu Scientific Instruments Inc., Columbia, MD

TP 444  LC-MS based analysis of the structural and functional roles of rRNA post-transcriptional modifications under photoxidative stress; Mariana B. P. Estevez1; Manasses Jora1; Scott Abernathy1; Patrick A. Limbach1; Balasubrahmanyam Addepalli1; 1Rieveschl 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; Rebecca Rose1; Olga Katsara1; Robert Banh1; Tenzin Lhakhan1; Manor Askenazi1; Robert Schneider1; Michael Pacold1; Drew Jones1; 1NYU 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; Kurokawa Yusaku1; Matsubara Yuki1; Masami Koike2; Yoshiho Yamauchi3; Taoka Masato3; Yokoi Yasuto1; Nakayama Hiroshi2; 1Mitsui Knowledge Industry, Tokyo, Japan; 2RIKEN Center for Sustainable Resource Science, Wako, Japan; 3Tokyo Metropolitan University., Hachioji, Japan

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TP 447  High throughput fine mapping of glycosylation enabled by DiLeuEN and ETD-MS; Miyang Li1; Lingjun Li2; 1University of Wisconsin Madison, Madison, WI; 2University 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; Dylan Nicholas T Tabang1; Philip B Emmerich2; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Division of Hematology and Medical Oncology, Department of Medicine, University of Wisconsin School of Medicine and Public Health, University of Wisconsin, Madison, WI; 3University of Wisconsin Carbone Cancer Center, Madison, WI; 4School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 5William S. Middleton Memorial Veterans Hospital, Madison, WI; 6McArdle 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; Thomas Schmitz1; Stuart Pengelly2; Eckhard Belau2; Diana Imhof3; Detlev Suckau2;
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1University Bonn, Protein Synthesis & Bioanalytics Core Facility, Bonn, Germany; 2Bruker Daltonics, Bremen, Germany

TP 450 Mass spectrometry-based data validation and machine learning models for citrullinome analysis; Raghothama Chaerkady1; Jared Delmar1; Wen Yu1; Yebin Zhou1; Gary P Sims1; Lisa H Cazares1; Sonja Hess1; 1R&D AstraZeneca, Gaithersburg, MD

TP 451 Retention Time Prediction for Phosphorylated Peptides in 2D HPLC-MS Proteomic Experiments; Taylor Battellino1; Darien Yeung2; Ying Lao3; Victor Spicer3; Helene Perreault1; Oleg Krokhin4; 1University of Manitoba/Department of Chemistry, Winnipeg, Manitoba; 2University of Manitoba, Winnipeg, MB; 3Manitoba Centre of Proteomics and Systems Biology, Winnipeg, MB; 4Manitoba 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 Fu1; John Muroski1; Hong Hahn Nguyen1; Robert P. Gunsalus1; Rachel R. Ogorzalek Loo1; Joseph A. Loo1; 1University 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. Bubis1; Lev I. Levitsky3; Mark V. Ivanov3; Mikhail V Gorschkov1; Irina A. Tarasova1; 1V.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 Kolibius1; David Avila1; Martin Ebeling1; Tom Dunkley1; Christine Hildebrandt2; Adrian Britschi2; Manuel Tzouros3; 1Roche Innovation Center Basel, Pharma Research and Early Development, Pharmaceutical Sciences, F. Hoffmann-La Roche Ltd., Basel, Switzerland; 2Roche 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. Bern1; Yong J Kil1; Abhishek Roushan1; Doron Kletter1; Claire J Bramwell1; Eric Carlson1; Guillaume Tremintin2; Christopher Adams2; Nagarjuna Nagaraj3; 1Protein Metrics Inc, Cupertino, CA; 2Bruker 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 Hubbard1; Ryan R. Julian1; 1University of California, Riverside, Riverside, CA

TP 457 Leveraging the extended instrument capabilities of a Tribrid MS using real-time PTM localization; William D Barshop1; Jesse D Canterbury1; Tony Zhao1; Romain Huguet1; Vlad Zabrouskov1; Graeme Mcalister1; 1Thermo 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 Buchanan1; Sara Carillo2; Angela Criscuolo3; Silvia Millan Martin2; Jennifer Sutton2; Phil J Widdowson1; Ken Cook1; Kai Scheffler1; Jonathan Bones2; 1Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; 2Roche Innovation Center Basel, Pharma Research and Early Development, Oncology Discovery and Translational Medicine Area, F. Hoffmann-La Roche Ltd., Basel, Switzerland; 3Thermo Fisher Scientific, Dreieich, Germany; 4Thermo Fisher Scientific, San Jose, California; 5Thermo Fisher Scientific, Germering, Germany

TP 459 Sequential phosphoproteomics and N-glycoproteomics of plasma-derived extracellular vesicles for breast cancer subtype biosignatures; Hillary Andaluz Aguilar1; I-Hsuan Chen1; J. Sebastian Paez1; Marco Hadasurya1; Anton B Iluk2; Guochen Qin1; Haiyang Zhang4; Chuan-Chih Hsu1; Sujin Li1; Jian-Kang Zhu1; Sonia Sugg2; Michael K. Wendl1; Haixu Tang5; Weizhou Zhang1; W. Andy Tao1; 1Purdue University, West Lafayette, IN; 2Tymora Analytical Operations, West Lafayette, Indiana; 3Shanghai Institute of Plant Stress Biology, Shanghai, China; 4School of Biological Sciences and Medical Engineering, Southeast University, Nanjing, China; 5Indiana University, Indianapolis, IN; 6University of Iowa, College of Medicine, Iowa City, Iowa; 7University 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 Stensballe1; Thomas Bouet Guldbæk Poulsen1; Christopher Abco1; Mikkel Eggert Thomsen1; Verena Tellstroem1; Dres Damgaard2; Claus Henrik Nielsen3; 1Aalborg University, Aalborg, Denmark; 2Bruker Daltonik GmbH, Bremen, Germany; 3Copenhagen University Hospital, Copenhagen, Denmark

TP 461 Quantitative analysis of in vivo methionine oxidation by heavy isotope labelling; John Q Bettinger1; Kevin A Welle1; Jennifer R Hryhorenko1; Sina Ghaemmaghami1; 1University of Rochester, Rochester, NY

PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS

TP 462 Optimizing enrichment of lowly abundant cellular retinol binding protein, type 1 (CRBP1) extracted from in-gel digest; Stephanie M Zalesak1; Wenjing Li1; Jianshi Yu1; Maureen A Kane1; 1University of Maryland School of Pharmacy, Baltimore, MD
TP 463  Absolute quantitation of peptides by Coulometric Mass Spectrometry using ferrocene tags; Praneeth Ivan Joel Fnu1; Hao Chen1; 1Department 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 Wang1; Wenpeng Zhang1, 2; Zheng Ouyang1; 1State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; 2Department 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 Balu-Rodriguez1; Daria Kucheraviaya1; Dilrukshika S. W. Palagama1; Apurva Lad1; Grace M. O'Neill1; Johnna A. Birbeck1; David J. Kennedy1; Steven T. Haller1; Judy A. Westrick1; Dragin Isailovic1; 1University of Toledo, Toledo, OH; 2Wayne State University, Detroit, MI

TP 466  QPREST+ validated isotope-labeled protein standard for absolute quantification using mass spectrometry; Åsa Makower1; Marie Utterbäck1; Tove Boström1; Gabriella Jensen1; Laura Pozzi1; Sofié Olander1; Ulrika Qundos1; Björn Forsström1; 1Atlas Antibodies AB, Stockholm, Sweden

TP 467  Large Therapeutic Peptide Quotient in Human Plasma Using a Highly Sensitive and Robust Assay with HILIC to RP 2D-LC-MS/MS; Moucun Yuan1; Meng Ye2; Yousef Basir1; Catherine Delguidice1; William R. Mylot1; Michael Cwik2; Mike Baratta2; 1PPD, Richmond, VA; 2Takeda 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 Woolfitt1; Maria I Solano1; Anne E Boyer1; John R Barr1; 1CDC, Atlanta, GA

TP 469  Highly sensitive quantitative analysis of Leuprolide from rat plasma using LC-MS/MS; Ashutosh Shelar1; Purushottam Sutar1; Shailendra anil Rane1; Bhaumik Trivedi1; Shailesh Damale1; Anant Lohar1; Deepthi Bhandarkar1; Navin Devadiga1; Ajit Datar1; Pratap Rasam1; Jitendra Kelkar1; 1Shimadzu Analytical (India) Pvt Ltd, Mumbai, India

TP 470  New PRM-PASEF for highly multiplexed targeted acquisition in clinical samples; Antoine Lesur1; Marta Mendes1; Jens Decker1; Sven Brehmer1; Schmit Pierre-Olivier1; Gunnar Dittmar1; 1Luxembourg Institute of Health, Strassen, Luxembourg; 2Bruker Daltonik GmbH, Bremen, Germany; 3Bruker Daltonik GmbH, Bremen, Germany; 4Bruker Daltonique S.A., Wissembourg, France

TP 471  High Sensitive Detection and Qualitative Analysis of therapeutic peptides using MRM Analysis; Faraz Rashid1; Dipankar Malakar1; Manoj Pillai1; 1SCIEX, 121, Udyog Vihar, Phase – IV, Gurgaon, Haryana, India

TP 472  Selective and sensitive quantification of glucagon in human plasma using microflow LC/Q-TOF MS; Tomoya Kudo1; Wataru Fukui1; Toshiya Matsubara1; 1Shimadzu Corporation, Kyoto, Japan

TP 473  Sample multiplexing with isotopic and isobaric TMT labeling for targeted pathway proteomics: application to aging mice; Qing Yu1; Haopeng Xiao2; Mark P Jedrychowski2; Devin K Schwepppe1; Jose Navarrete-Perrera1; Jeffrey Knott1; John C Rogers1; Edward T Chouchani2; Steven P Gygi1; 1Harvard Medical School, Boston, MA; 2Thermo Fisher Scientific, Rockford, IL

TP 474  Utilizing Differential Ion Mobility– Mass Spectrometry for Improved Immunopeptide Detection; Elyssa Alvarez1; Tavleen K. Kochar1; James E. Keating1; Shengjie Chai1; Benjamin G. Vincent1; Sally A. Hunsucker1; Paul M. Armistead2; Gary L. Glish1; 1Department of Chemistry & Environmental Science, New Jersey Institute of Technology, Newark, NJ; 2State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China

TP 475  Quantitative analysis of Ras and AKT signaling pathways using a SureQuant targeted MS workflow; Bhavin Patel1; Penny Jensen1; Aaron S Gajadhar1; Sebastien Gallien1; Andreas Huhmer2; Daniel Lopez-Ferrer2; Kay Opperman1; Ryan Bomgarden1; John C Rogers1; 1Thermo Fisher Scientific, Rockford, IL; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA

TP 476  Glycosylation improves stability of neuropeptides and elevates blood brain barrier (BBB) penetration; Chenxi Liu1; Mitchell J. Bartlett1; Christopher R. Apostol1; Lajos Szabo1; Robin Poit1; Torsten Falk2; Michael L. Heien1; 1Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ; 2Department of Neurology, The University of Arizona, Tucson, AZ; 3Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ

TP 477  A novel, simple and sensitive LC-MS/MS method for simultaneous quantification of insulin glargine and its metabolites (M1 and M2); Avinash B Gaikwad1; Atmakuri Chaitanya Krishna1; Yogesh Gorakhnath Arote1; Sujit Bhaskar Patil1; Jitendra Kelkar2; Ajit Datar2; Pratap Rasam2; 1Shimadzu Application Development Centre, Navi Mumbai, India; 2Shimadzu Analytical (India) Pvt Ltd, Marol, Andheri, Mumbai, India
TUESDAY POSTERS (TP) Pages 45-85 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

TP 480 Improving depth of coverage and absolute peptide detection limits using FAIMS separation coupled to a quadrupole-Orbitrap mass spectrometer; Amirmansoor Hakimi1; Tabiwang N. Arrey2; Josh Nicklay3; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 3Thermo Fisher Scientific, Somerset, NJ

TP 481 Quantitation and Identification of Peptides by Free Radical Isobaric Tags for Relative and Absolute Quantitation; Edgar M Manriquez1; Jinshan Gao2; 1Montclair State University, Montclair, NJ; 2Montclair 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 Mori1; Tomohiro Kohata1; Ryoitaro Yagi1; Yui Kaneko1; Takeshi Masuda1; Shingo Itô1; Sumio Ohtsuki1; 1Kumamoto 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 Mu1; Yue Huang1; Anton I Rosenbaum1; 1Clinical Pharmacology & Quantitative Pharmacology, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, South San Francisco, California

PROCESS DEVELOPMENT MS
TP 484 Industry-wide Performance of the New Peak Detection Component of the Multi-Attribute Method; Trina Mouchahoir1, 2; John Schiel1; 2; Rich Rogers3; 1National Institute of Standards and Technology, Gaithersburg, Maryland; 2Institute for Bioscience and Biotechnology Research, Rockville, Maryland; 3Bristol-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 Lame1; Lindsay Hatch1; Dave Highton3; 4; Paul Rainville1; Gordon Fujimoto2; 1Waters Technologies Corporation, Milford, MA; 2Waters Technologies Corporation, Beverly, MA; 3Waters Technologies Corporation, Milford, MA; 4Waters Technologies, Wilmslow, United Kingdom

TP 487 Making LC-MS Sensibly Useful for Host Cell Protein Applications; Amy J Claydon1; St John Skilton2; A. Michelle English3; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Protein Metrics, Inc., Cupertino, CA; 3Protein Metrics Inc., Cupertino, CA

TP 488 Refinement of HR Multi-Attribute Method from Sample Preparation to Data Analysis; Haichuan Liu1; Hao Yang1; Min Du1; 1Thermo 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 Blakeman1; Ji Young L Anderson1; Colin M Gavin1; Kerin E Gregory1; Scott E Miller3; Glenn A Harris1; 1908 Devices, Inc., Boston, MA

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY
TP 490 Hydroxyl-Radical Reaction Pathways for the Fast Photochemical Oxidation of Proteins Platform As Revealed by 18O Isotopic Labeling; Roger (xiaoran) Liu1; Mengru Mira Zhang1; Bojie Zhang1; Don L. Rempel1; Michael L. Gross1; 1Washington University in St. Louis, St. Louis, MO

TP 491 Ligand and Metal Binding to Wild Type and Mutant α-Synuclein; Jaybree Lopez1; Carter Lantz1; Rachel R. Ogorzalek Loo1; Joseph A. Loo1; 1University 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 Technology, Beijing, China

TP 493 Protein structural accessibility differences associated with Alzheimer’s disease in cerebrospinal fluid by limited proteolysis-mass spectrometry; Danielle A Faivre1; Eric L Huang2; Michael J MacCoss3; 1University of Washington, Seattle, WA; 2Washington University in St. Louis, St. Louis, MO; 3Washington University School of Medicine, St. Louis, MO

TP 494 Fast Footprinting of proteins with Carbocations: The Hydrophobic Trifluoromethoxy benzyl carbocation; Jie Sun1; Xiaoran Liu2; Chunyang Guo2; Shuang Li3; Weikai Li3; Michael L. Gross2; 1Washington University in St. Louis, St. Louis, MO; 2Washington University in St. Louis, St. Louis, Missouri; 3Washington University School of Medicine, St. Louis, MO

TP 495 In-Depth Structural Analysis of G Protein-Coupled Receptors through Cross-Linking Mass Spectrometry; Lisha Xia1; Ziliang Ma4; Jiahui Tong1; Yuliang Tang2; Wenqing Shui1, 3; 1ShanghaiTech University, Shanghai, China; 2Peking University, College of Chemistry, Beijing, China; 3Human Institute, ShanghaiTech University, Shanghai, China
TP 496  Delineating Metal-Mediated vs. Direct Protein Oxidation Pathways: Implications for Oxidative Modification Mapping in Metalloproteins; Victor Yin1; Derek Holzschwerdt1; Lars Konermann1; 1University 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 Sipe1; Kevin Jeanne Dit Fouque2; Alyssa Garabedian2; Fenfei Leng2; Francisco Fernandez-Lima4; Jennifer S Brodbelt1; 1University of Texas at Austin, Austin, TX; 2Florida 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. Brit1; Tristan Cragnoni2; Chris Hughes3; Johannes P. C. Vissers3; Konstantinos Thalassinos1; 1University College London, London, London, United Kingdom; 2Birkbeck College, University of London, London, United Kingdom; 3Waters Corporation, Wilmslow, United Kingdom

TP 499  TMT-labeling assisted profiling of protein structure in human brain tissue of Alzheimer’s disease; Kaiwen Yu1; Mingming Niu1; Hong Wang1; Yuxin Li1; Zhiping Wu1; Junmin Peng1; 1St. Jude Children’s research hospital, Memphis, TN

TP 500  Who’s in charge: how metal ions define α-synuclein structure; Rani Moons1; Albert Konijnenberg1; Anne-Marie Lambeir1; Frank Sobott1; 1University of Antwerp, Antwerp, Belgium; 2University of Leeds, Leeds, United Kingdom

TP 501  CCS measurements of low-charged (z < 3) electrosprayed proteins; Ben Aguilar1; W Henry Benner1; 1Ion DX, Inc., Monterey, CA

TP 502  Investigating the Impact of Heparan Sulfate Domain Structure on Interleukin 8 Heparan Sulfate interactions; Robert V Williams1; Tanvir Ahmed1; Pradeep Chopra1; Lifeng Sun2; Geert-Jan Boons3; I. Jonathan Amster1; 1University of Georgia, Athens, GA; 2Utrecht University, Utrecht, Netherlands; 3Complex Carbohydrate Research Center, University of Georgia, Athens, GA

TP 503  Mass Spectrometry-based Characterization of Protein Structural Disruption Under Mechanochemical Stress Conditions; Jazmine Crain1; Balasubrahmanyan Addepalli1; James Mack1; 1University of Cincinnati, Cincinnati, OH

TP 504  Measurement of the Stability of Immunoglobulin G Two by Cyclic Ion Mobility Spectrometry; Kyle Buckley1; Lucas W Henderson1; Edie M Sharon1; David E. Clemmer1; 1Indiana University, Bloomington, IN

TP 505  Post-translational Modifications and Their Effects on the Conformation and Function of Hsp90 in Embryonic Stem Cells; Seth W Mcnutt1; Feixia Chu1; Daniel T Thornton1; Hieu Nguyen1; 1University 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 Nash1; Tyler Marcinko1; Richard W Vachet2; 1University of Massachusetts Amherst, Amherst, MA; 2University 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: Hong Hee Song1; Jing Yan1; Nicole D. Wagner1; Aaron Balog1; Jing Li2; Richard Huang2; John Newitt2; Mark Witmer2; Louis Lombardo2; Olafur Gudmundsson2; Guodong Chen2; Gross L. Michael1; 1Washington University, St. Louis, MO; 2Bristol-Myers Squibb Company, Princeton, NJ

TP 508  Domain orientation of the HS-binding protein Robo1 studied by IM-MS, NMR, and SAXS; Robert Williams1; Jeong Y Yang2; Yunyun Gao2; Arwen Pearson2; Kelley Moremen2; James Prestegard2; Jon Amster1; 1University of Georgia, Athens, GA; 2Complex Carbohydrate Research Center, University of Georgia, Athens, GA; 3University of Hamburg, Hamburg, Germany

TP 509  Characterization of Common Human Histones using nESI-CIA-TIMS-MS; Yasir Mamun1; Khoa Ngoc Pham1; Francisco A. Fernandez-Lima1; 1Florida International University, Miami, FL

TP 510  Conformational Analysis of Mtr4 using Hydrogen-Deuterium Exchange; Naifu Zhang1; Keith J Olsen2; Sean J Johnson2; Sheena D’arcy3; 1UT Dallas, Richardson, TX; 2Utah State University, Logan, UT; 3UT Dallas, Richardson

TP 511  Structure-based validation can drastically under-estimate error rate in proteome-wide cross-linking mass spectrometry; Haiyuan Yu1; Yugandhar Kumar1; Ting-Yi Wang1; Elnur Elyar Shayhidin1; 1Cornell University, Ithaca, NY

TP 512  Evidence in glioma that Ghost proteins are functional Regulators using large scale crosslink mass spectrometry and TurboID; Tristan Cardon1; Etienne Coya1; Estelle Laurent1; Julien Franck1; Michel Salzet1; Isabelle Fournier1; 1PRISM, InsermUT1192, Villeneuve d’ascq, France

TP 513  Modeling of a Sin3/HDAC Complex Sub-structure Using Crosslinking Mass Spectrometry (XL-MS); Charles A.S. Banks1; Yin Zhang1; Sayem Miah1; Yan Hao1; Mark K Adams1; Zhihui Wen1; Janet L Thornton1; Laurence Florens2; Michael P. Washburn1; 1Stowers 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 Capua1; Blake E. Szkoda1; Venkat Golapalan1; Vicki H Wysocki1; 1The 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 Jain1; Khaja Muneeruddin2; Jeremy Anderson3; Michael J Harms3; Scott A Shaffer2; C. Robert Matthews2; 1Case Western Reserve University, Cleveland, OH; 2University of Massachusetts Medical School, Worcester, MA; 3University of Oregon, Eugene, OR

TP 516  Measuring protein conformational change in living cells by quantitative, comprehensive, and ultra-sensitive protein footprinting; Jenna G. Caldwell1; Bjorn-Erik Wulff1; Lichao Zhang2; Joshua E. Elias2; Pehr A. B. Harbury1; 1Biochemistry, Stanford University School of Medicine, Stanford, CA; 2Chan Zuckerberg BioHub, Stanford, CA

PROTEOMICS: CLINICAL APPLICATIONS I

TP 517  The Prostate Cancer in vivo Secretome; Amanda Khoo1; Joseph J. Otto2; Andrew Maclin3; Zhuyu Qu1; Vladimir Ignatchenko2; Katharina Fritsch1; Lydia Y. Liu1; Meinusha Govindarajan1; Danny Vespri1; Julius O. Nyawidhe1; Stanley Liu1; O. John Semmes1; Paul C. Boutros1, 4; Thomas Kislinger3; 1Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; 2Division of Pathology, Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA; 5Sunnybrook 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 Peng1; Jie Jiang2; Chunling Wan2; 1National Facility for Protein Science, Zhangjiang Lab, SARI, CAS, Shanghai, 201210, China; 2Shanghai 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 Sanford1; Maria F Pino2; Marina A Gritsenko2; Chelsea M Hutchinson1; Joshua R Hansen1; Ronald J. Moore1; Wei-Jun Qian1; Lauren M Sparks2; Joshua N Adkins1; Paul Piechowski1; 1Pacific Northwest National Lab, Richland, WA; 2AdventHealth, Orlando, FL

TP 521  PQ500 and SureQuant enables highly reproducible absolute quantification of 500 plasma proteins for clinical studies; Jan Muntel1; Tejas Gandhi1; Hui Li1; Asim Shekpor1; David Yowe1; Jasison Jacob1; William Chutkow1; Karen Wang1; Sebastian Müller1; Yuehan Feng1; Roland Bruderer1; Lukas Reiter1; Biognoys, Schlieren, Switzerland; 2Novartis 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 Mitsa1, 2; Christophe Goncalves3; Adriana Aguilar-Mahecha1; Qianyu Guo1, 3; Mark Basik1, 4; Alan Spatz2; Gerald Batist1, 3, 6; Wilson H. Miller, Jr.1, 3, 7; Sonia V. Del Rincon1, 3; René Zahedi2; Christoph H. Borchers2, 3, 8; 1Division of Experimental Medicine, McGill University, Montreal, QC; 2Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; 5Department of Pathology, Segal Cancer Centre, Montreal, QC; 6Department of Pathology, Jewish General Hospital, McGill University, Montreal, QC; 7Rossy Cancer Network, McGill University, Montreal, QC; 8Exactinn Innovation, Montreal, QC; 9Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia

TP 524  Proteomic profiling of glycosylated serum proteins; Yavor Vazmitsev1; Shawn Connolly1; Kuanysheva Kabytaev1; 1University 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 Do1; Hyunsoo Kim2; Injoon Yeo2; Jihyeon Lee2; In Ae Park2; Han Suk Ryu2; Youngsoo Kim1, 2; 1Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea; 2Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, South Korea; 3Department 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-Jankovic1; Sandra Gaisbauer2; Goran Mitulovic1; 1Medical University of Vienna, KILM, Vienna, Austria; 2Clinical Institute of Laboratory Medicine, Vienna General Hospital, Vienna, Austria

TP 527  Next generation potential biomarker candidates for Plasmodium vivax: Alternative to existing RDT?; Shalini Aggarwal1; Apoorva Venkatesh1; Jayanthi Shastri1; Swati Patankar1; Sanjeeva Srivastava1; 1Indian Institute of Technology, Bombay, Mumbai, India; 2T N Medical College & Nair Hospital, Mumbai, India; 3IIT Bombay, Mumbai, India
In-depth serum profiling revealing novel protein biomarkers associated with Bechet disease diagnosis and therapy; Linlin Cheng1,2; Dongxue Wang1; Guibin Wang5; Ziyan Wu3; Meng Xu4; Xiaomei Zhang2; Liubing Li1; Chenxi Liu1; Jiayu Dai2; Songxin Yan1; Fuchu He2; Fengchun Zhang2; Xiaobo Yu2; Yongzhe Li1; 1Peking Union Medical College Hospital, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing, China; 2State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences, Beijing Institute of Lifeomics, Beijing, China; 3Peking Union Medical College Hospital, Peking Union Medical College and Chinese Academy of Medical Sciences, Key Laboratory of Rheumatology and Clinical Immunology, Beijing, China

Multi-stage analysis of high-resolution mass spectrometry data reveals novel antimicrobial peptides (AMPs) in the cerebrospinal fluid of Alzheimer patients; Satya Saxena1; Abhay Moghekar2; David R Goodlett1; 3; 1University of Maryland School of Dentistry, Baltimore, MD; 2Department of Neurology, Johns Hopkins University School of Medicine, Baltimore, MD; 3University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland

Proteomic Analysis of Exosomes Secreted During Epithelial to Mesenchymal Transition in Ovarian Cancer; Carolina Thome1,2; Germano Ferreira1,2; Guilherme Lanfredi1; Francisco CJ Reis2; Marcus Smolka2; Vitor Faca1,2; 1Center for Cell Based Therapy - University of Sao Paulo, Ribeirao Preto, Brazil; 2Ribeirao Preto Medical School - University of Sao Paulo, Ribeirao Preto, Brazil; 3Well Institute for Cell and Molecular Biology - Cornell University, Ithaca, NY

Simplified Sample Preparation Strategy for Plasma Proteomics and its Application to a Pilot Study of Ischemic and Non-Ischemic Cardiomyopathy Patients; Meghan J. Mcfadden1,2; Esha Joshi3; Douglas S. Lee1,4,5; 1Department of Neurology, University of Tennessee Health Science Center, Memphis, TN; 2Center for Inflammatory Cardiovascular Disease, University of Tennessee Health Science Center, Memphis, TN; 3Department of Pathology, Seoul National University Hospital, Seoul, South Korea; 4Department of Surgery, Seoul National University College of Medicine, Seoul, South Korea; 5Department of Preventive Medicine, Seoul National University College of Medicine, Seoul, South Korea

A multi-omic surfaceome study identifies DLK1 as an epigenetically regulated protein and immunotherapeutic target in neuroblastoma; Amber K. Weiner1,2; Alexander B. Radaoui2; Matthew Tsang2; Dan Martinez2; Simone Sidoli2; Karina L. Conkrite2; Alberto Delaide2; Jo Lynne Rokita2; Maria V. Lane2; Zaiman Vaksman2; Komal S. Rathi3; Pichai Raman2; Liubing Li1; 1Department of Pathology, Seoul National University College of Medicine, Seoul, South Korea; 2Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; 3Proteomics Core Facility, Biomedical Research Institute, Seoul National University College of Medicine, Seoul, South Korea

In depth proteomics of the kidneys from autoimmune type I diabetes rat model through MALDI - Imaging Mass Spectrometry; Konomi Uchida1; Yume Mukasa1; Kazuhiko Ishibashi1; Yuki Kuzuhara1; Takashi Nirasawa2; Ryo Kajita1; Hiroki Yanagi2; Nobuto Kakuda1; Masaya Ikegawa1; 1Doshisha university, Faculty of Life and Medical Sciences, Kyoto, Japan; 2ONO Pharmaceutical Co., Ltd., Fukui, Japan; 3Bruker Japan K.K., Yokohama, Japan

A multiplex targeted Mass spectrometry approach for the quantification of synuclein proteoforms in human biological fluids; Marie-Laure Pons1,2; Jerome Vialaret1; Stephane Moreau2; Sylvain Lehn1; Charlotte Macron1; Matthieu Porchet1; James Holzwarth2; Joy Richard3; Giulia Lizzo3; Philipp Gut1; Loic Dayon1,2; 1Department of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA; 2Children's Hospital of Philadelphia, Philadelphia, PA; 3Albert Einstein College of Medicine, Bronx, NY; 4British Columbia Cancer Agency, Vancouver, BC; 5Keck School of Medicine of USC, Los Angeles, CA; 6National Cancer Institute, Bethesda, MD; 7RTI International, Research Triangle Park, NC; 8University of Pennsylvania, Philadelphia, PA; 9ADC Therapeutics (UK) Ltd, London, United Kingdom

A combined proteomic and proteogenomic strategy helps decipher the zebrafish proteome; Charlotte Macon1; Matthieu Porchet1; James Holzwarth2; Joy Richard3; Giulia Lizzo3; Philipp Gut1; Loic Dayon1,2; 1Proteomics, Nestlé Institute for Food Safety & Analytical Sciences, Nestlé Research, Lausanne, Switzerland; 2Genomics, Nestlé Institute for Food Safety & Analytical Sciences, Nestlé Research, Lausanne, Switzerland; 3Cell Biology, Nestlé Institute of Health Sciences, Nestlé Research, Lausanne, Switzerland; 4Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Multiproteomic approaches to study the epithelial-to-mesenchymal transition; Paola Cavaliere1; Noah E. Dephoure1; 1Weill Cornell Medical College, New York, NY
TP 538  Proteome-wide detection of drug-target engagement with chaperone-dependent protein destabilization and degradation; Taylur Ma1; Kelvin F Cho2; Christopher Rose3; Donald Kirkpatrick1; Robert Blake4; Kebing Yu5; 1Genentech Inc., South San Francisco, CA; 2UC Berkeley, Berkeley, CA

TP 539  Deep nanogram-scale proteome profiling by isobaric labeling, extensive liquid chromatography, and mass spectrometry; Danling Liu1; Jeffrey M. Sifford1; Zhiping Wu1; Boer Xie1; Kanisha Kavdia1; Kaiwen Yu1; Shu Yang1; Junmin Peng1; 2St Jude Children’s Research Hospital, Memphis, TN

TP 540  Comparison of Proteomic Analysis of Exosomes Purified Using Traditional Ultracentrifugation vs. Dialysis Concentration and Electrophoresis; Elizabeth R Nunn1; James Wareham1; James N. Higginbotham2; Jeffrey Franklin2; Dennis K. Jeppesen3; Victor Pramov4; Siddarth Pratap5; Robert J Coffey6; Amy-Joan L. Ham6; 1Belmont University, Nashville, TN; 2Vanderbilt University Medical Center, Nashville, TN; 3Meharry Medical College, Nashville, TN

TP 541  Electron Transfer Dissociation Technique for Human Serum Albumin Adductomics; Stanislaw Stanishevskii1; Monica L V Maier1,2; Yury Vasilev1,2; David Williams1,2; Dr. Claudia Susanne Maier1,2; 1Oregon State University, Corvallis, Oregon; 2Linus Pauling Institute, Corvallis, Oregon

TP 542  Optimization of 16-plex Tandem Mass Tag Mass Spectrometry for large-scale proteomics; Zhen Wang1; Kaiwen Yu1; Haiyan Tan1; Zhiping Wu1; Ji-Hoon Cho1; Xian Han1,2; Thomas G. Beach1; Junmin Peng1; 1St Jude Children’s Research Hospital, Memphis, TN 38105; 2University of Tennessee Health Science Center, Memphis, TN 38163; 3Banner Sun Health Research Institute, Sun City, AZ 85351

TP 543  Integration of Nuclear Acid Extraction from Tissue Samples Into Standard Mass Spectrometry-Based Proteomic Workflows for Multi-’Omic Analysis of Clinical Samples; Sandra E. Spencer Miko1; Ryan Riley1; Grace Cheng1; Karina Neilson1; Gian Luca Negri1; Aaron H. Gillmor2; Ted Verhey2; Sorana Morriessy3; Gregg B. Morin1,2; 1Canada’s Michael Smith Genome Sciences Centre, Vancouver, BC; 2University of Calgary, Calgary, AB

TP 544  Improving Proximity-labeling Proteomics Approach to Study Protein-protein Interactions; Ashley M. Frankenfield1; Ling Hao1; 1George Washington University, Washington, DC

TP 545  A Method of High-Purity Extracellular Vescicle Enrichment from Microliter-scale Human Serum for Proteomic Analysis; Xiaohui Ji1,2; Sisi Huang3; Jie Zhang4; Zhijing Tan5; Yu Lin6; R. Kenneth Marcus1; Jianhui Zhu1; David M Lubman1; 1University of Michigan, Ann Arbor, Michigan; 2Chongqing University Cancer Hospital, Chongqing, China; 3Clemson University, Clemson, SC

TP 546  Two Dimensional Mass Spectrometry (2DMS): How Far Can We Go in Proteomics?; Yuko Pui Yiu Lam1; Christopher A. Wootton1; Tomos E. Morgan1; Bryan P. Marzullo1; Cookson K. C. Chiu1; Alina Theisen1; Remy Gavard1; Meng Li1; Mark P. Barrow1; Peter B O’Connor1; 1University 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 Villacob1; Luke Richardson1; Fabrizio Donnarumma2; Kermit K Murray2; Touradj Kermit1; 1Baylor University, Waco, TX; 2Louisiana State University, Baton Rouge, LOUISIANA

TP 548  Analysis of Metalloproteins in Pseudomonas aeruginosa Using Online Comprehensive Two-dimensional Active Modulation Liquid Chromatography; Matthew Mcilvin1; Mak Saito1; 1Woods 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. Neely1; Magnus Palmblad2; Phillip A. Wilmarth2; Alison M. Bland4,5; Michael G. Janech4,5; 1National Institute of Standards and Technology, Charleston, SC; 2Leiden University Medical Center, Leiden, Netherlands; 3Oregon Health & Science University, Portland, Oregon; 4College of Charleston, Charleston, SC; 5Hollings Marine Laboratory, Charleston, SC

TP 550  Proteolytic resistant streptavidin increases dynamic range in affinity purification mass spectrometry workflows; Jessica Read1; Ansarq Brock1; Jan Grunewald1; Shima Rayatpisheh1; John Venable1; Ajay Vashisht1; 1Genomics 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. Bergo1; Ghaith Hamza2,3; Serge DiKler4; Abhay Moghekar5; Sergey Mamaev1; Manor Askenazi1; Don M. Wojchowski1; Camilla Worsfold1; Jeffrey C. Silva1; 1ADEPTRIX CORP., Beverly, MA; 2AstraZeneca, BioPharmaceuticals R&D, Discovery Sciences, Boston, MA; 3University of New Hampshire, Durham, NH; 4Bruker Scientific LLC, Billerica, MA; 5Johns Hopkins University School of Medicine, Baltimore, MD; 6Biomedical 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 Lilla1; Samuel Atkinson1; Jiska Van Der Reest1; Lisa Neilson1; Sara Rossana Zanivan1; 1The Beatson Institute for Cancer Research, Glasgow, United Kingdom
TP 554  A Proline- and Alanine-specific protease is complementary to trypsin in proteomics applications; Diana Samodova1; Chris Hosfield2; Christian Necip Cramer3; Maria Valeria Giulii4; Giulia Franciosa1; Enrico Cappellini5; Michael Rosenblatt2; Christian Dahl Kelstrup3; Jesper Velgaard Olsen1; 1Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; 2Promega Corporation, Madison, WI; 3Novo Nordisk A/S, Måløv, Denmark; 4University of Rome, Rome, Italy; 5Natural 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 Aibara1; Mikirou Nakashima1; Naotaka Kuroda1; Kaname Ohyama1; 1Nagasaki University, Nagasaki, Japan

TP 556  Sample Preparation by Easy Extraction and Digestion (SPEED) - A Universal, Rapid, and Detergent-free Protocol for Proteomics; Joerg Doellinger1; Andy Schneider1; Marcel Hoeller1; Peter Lasch1; 1Robert Koch-Institute, Centre for Biological Threats and Special Pathogens, Proteomics and Spectroscopy (ZBS6), Berlin, Germany
### PROTEOMICS: QUANTITATIVE I

| TP 557 | Systematic evaluation of protein synthesis inhibition through global quantification of newly synthesized proteins; Ming Tong¹; Suttipong Suttapitugsakul¹; Senhan Xu¹; Ronghu Wu¹; ¹Georgia Tech, Atlanta, GA |
| TP 558 | In-depth proteome coverage and stoichiometric quantification of thiol-based redox modifications in mammalian tissues; Tong Zhang²; Matthew J. Gaffrey¹; Karl K. Weitz¹; Ronald J. Moore¹; Wei-Jun Qian¹; ¹Pacific Northwest National Lab, Richland, WA |
| TP 559 | Label-free quantitative method for proteomics using one top peak intensity of peptides; Ki Na Yun¹,²; Heeyoun Hwang¹; Geul Bang¹; Gun Wook Park¹; Hye-Jung Kim³; Eugene Lee¹; Yong-In Kim³; Jeong Hee Moon⁵; Sungho Yun¹; Jong Shin Yoo¹; Jin Young Kim¹; ¹Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; ²Department of Chemistry, Sogang University, Seoul, South Korea; ³K-bio health, Osong, South Korea; ⁴Korea Research Institute of Standards and Science (KRISS), Daejeon, South Korea; ⁵Disease Target Structure Research Center, KRIIB, Daejeon, South Korea |
| TP 560 | A Comprehensive Evaluation of Variabilities Arising from Experimental Factors on LC-MS-based Proteomics Biomarker Discovery; Min Ma¹,²; Shichen Shen¹,³; Shihan Huo¹; Ming Zhang¹,³; Jun Qu¹,³; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Institute, Buffalo, NY; ³New 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 Dupree¹; Bernard Crimmisa¹; Thomas Holsen¹; James Pagano²; Brooke Thompson²; Krista Christensen²; Michelle Raymond³; Jonathan Meiman³; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²SUNY Oswego, Oswego, NY; ³Wisconsin Department of Health Services, Madison, WI |
| TP 562 | Presynaptic protein dysfunction in the initial stages of amyloid proteotoxicity; Timothy Hark¹; Nalini R Rao¹; Jeffrey Savas¹; ¹Northwestern 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 Islam¹; Michelle Gadush¹; Maria D. Person¹; Mona C Mehdy¹; ¹University 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 Tawalbeh¹,²; Tchilabalo D Alayi¹; Emily Canessa¹; Mansi V Goswami¹; Yetrib Hathout¹; ¹School of Pharmacy and Pharmaceutical Sciences, State University of New York at Binghamton, Johnson City, New York; ²Biomedical 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 Rasam¹,²; Shichen Shen²,³; Shuo Qian²,⁴; Jun Qu¹,²,³,⁴; ¹Department of Biochemistry, University at Buffalo, Buffalo, New York; ²Center of Excellence in Bioinformatics and Life Sciences, Buffalo, New York; ³Department of Pharmaceutical Sciences, University at Buffalo, Buffalo, New York; ⁴Department 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 Mosen¹; Roman Saksorn¹; Robert Hardt¹; Biswajit Moharan¹; Edgar Kaade¹; Thomas Ruppert²; Volkmar Gieselmann¹; Dominic Winter¹; ¹Institute for Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany; ²Centre for Molecular Biology of Heidelberg University, Heidelberg, Germany |
| TP 567 | Disruption-Compensation (DisCo) Analysis of RNA Polymerase II Interactome in Phosphatase Mutant; Katlyn H Burris¹; Whitney R Smith-Kinnaman¹; Guihong Qi¹; Amber L Mosley¹; ¹Indiana University School of Medicine, Indianapolis, IN |
| TP 568 | Multiplexed quantitative proteomics analysis of Human Brain Organoids; Anita Saraf¹; Chongbei Zhao¹; Michaela E. Sardu¹; Gaye Hattem¹; Tari J Parmely¹; Laurence Florens¹; Michael P. Washburn¹,²; ¹Stowers Institute for Medical Research, Kansas City, MO; ²Department 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 Rasam¹,²; Brian R. Weil³; ¹Department of Biochemistry, State University of New York, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, NY; ³Department of Physiology and Biophysics, Buffalo, NY; ⁴Clinical and Translational Research Center, Buffalo, NY; ⁵Department of Medicine Jacobs School of Medicine & Biomedical Sciences, Buffalo, NY; ⁶Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY |
| TP 570 | Differentially Activated Signaling Pathways in Lymphatic Anomalies Cells; Jong Min Choi¹; Feng Jin¹; Antrix Jain¹; Alexander B. Saltzman¹; Anna Malovannaya¹; Wa Du¹; Thuy Phung¹; Sung Yun Jung¹; ¹Baylor 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 Yaw Wong1; Kin Leung Kwan2; Henry H. N. Lam1; 1Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Kowloon, China; 2Division 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 Akter1; Srigayatri Ponnavaiyan1; Bianca Kögl-Mohrbacher2; Florian Bleibaum3; Markus Dämme3; Bernhard Y Renard4; Dominic Winter1; 1Institute for Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany; 2Bioinformatics Unit (MF1), Robert Koch Institute, Berlin, Germany; 3Institute for Biochemistry, University of Kiel, Kiel, Germany; 4Hasso Plattner Institute, University of Potsdam, Potsdam, Germany

TP 573  Understanding Cell Competition using Mass Spectrometry:  
Suniya Khatun1; Konstantinos Thalassinos1; 1University College London, London, United Kingdom

TP 574  An anomalous low codeine result linked to poppy seed ingestion solved by HRMS data analysis:  
Ana Celia Grenier1; Phillip Hackett1; Lawrence J. Andrade1; 1Dominion 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;  
Annelinde Damont1; Vivian Delcourt2; Stéphane Trevisiol2; Yves Moulot2; Patrice Garcia4; Ludovic Baille-Chouriberry2; Christophe Junot1; François Fenaille1; Jean-Claude Tabet1, 3, 4Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France; 2GIE-LCH, Laboratoire des Courses Hippiques, Verrières-le-Buisson, France; 3Sorbonne 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. Rennie1; Frank Kuhlmann1; James S. Pyke1; Stephen Madden1; O. David Sparkman2; 1Agilent Technologies, Santa Clara, CA; 2University of the Pacific, Stockton, CA

TP 577  An efficient approach to oligomer extraction from extractables using single-use systems:  
Emily Volk1; Bin Sun1; Rolf Kern2; Owen Perlowski2; Benben Song1; 1Pall Corporation, Westborough, MA; 2SCIEX, Redwood Shores, California 1201

TP 578  ms.epfl.ch on-line tool, new functionalities:  
Daniel Ortiz1; Natalia Gasilova1; Francisco Sepulveda1; Luc Patiny1; Laure Menin1; 1EPFL, 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 Sekar1; Aman Sharma1; Sandeep Choudhary1; Manoj G Pillai1; 1ScieX, 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 Teran1; Yufei Chen1; Xinyi Sui1; Tim Stratton2; Nelson Vinueza1; 1North Carolina State University, Raleigh, NC; 2Thermo 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 Pavlov1; Sihang Xu1; Kipling Will2; Brandt Weary2; Athula B. Attygalle1; 1University of Chinese Materia Medica, Shanghai University of Traditional Chinese Medicine, Shanghai, China; 2Waters Corporation Shanghai Science & Technology Co Ltd, Shanghai, China

TP 582  Monitoring Enzymatic Reactions by LC/Single Quad to Gain Insights on Reaction Mechanisms:  
Kyle J Covert1; Carim Van Beek2; 1Agilent Technologies, Santa Clara, CA; 2University of the Pacific, Stockton, CA

TP 583  Integrated qualitative analysis of volatile compounds from beer by using SPME-GC-HRTOFMS with EI/ElF;  
Koji Okuda1; Michael C Long2; Lynda McMaster-Schuyler2; Jacob T Shelley2; A John Dane1; Robert B Cody1; 1EPFL, Lausanne, Switzerland; 2University of the Pacific, Stockton, CA

TP 584  A fast screening approach based on SONAR acquisition and UNIFI library for hepatotoxic pyrrolizidine alkaloids from herbal medicines and preparations:  
Feng Xiong1; Aizhen Xiong1; Yanchoo Shi2; Ming Yuan2; Kate Yu1; Li Yang1; Zhengtao Wang1; 1Institute of Chinese Materia Medica, Shanghai University of Traditional Chinese Medicine, Shanghai, China; 2Waters Corporation Shanghai Science & Technology Co Ltd, Shanghai, China

TP 585  A case study of the MassChemsite Reaction Tracking workflow: detecting and identifying byproducts during PROTAC synthesis:  
Laura Goracci1; Elisabeth Ortega-Carrasco2; Ismael Zamora2, 3; Fabien Fontaine2; Jenny Desantis1; 1Department of Chemistry, Biology, and Biotechnology, University of Perugia, Perugia, Italy; 2University of Perugia, Perugia, Italy; 3Institute for Biochemistry and Molecular Biology, University of Perugia, Perugia, Italy
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

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; 2; Samir Vyas; 2; Agilent Technologies, BENGALURU, India; 2; Agilent Technologies, Mumbai, India

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; University of Florida Department of Chemistry, Gainesville, FL; 2; St. Louis University Department of Physiology and Pharmacology, St. Louis, MO

Selective Pulse Chase-SILAC Labeling of Three-Dimensional Multicellular Spheroids for Global Proteome Analysis; Nicola C. Beller; 1; Jessica K. Lukowski; 2; Amanda B. Hummon; 1; The Ohio State University, Columbus, OH; 2; University of Notre Dame, Notre Dame, IN

Vascular beds proteome dynamics in vascular dysfunction induced by an acute inflammatory response; Aida Serra; 1; Xavier Gallart-Palau; 1, 2; Pec Proteomics, IMDEA Food Research Institute, Madrid, Spain; 2; IISPV, Hospital Universitari Institut Pere Mata, Reus, Spain

TMTpro16plex Reagents Reach New Sample Multiplexing Heights at Proteome-scale Depths in Quantitative Proteomics; Jiaming Li; 1; Jonathan Van Vranken; 1; Laura Pontano Vaites; 1; Devin Schweppe; 1; Edward L Hutlin; 1; Chris Etienne; 2; Premchendar Nandhikonda; 2; Rosa Viner; 2; Aaron M Robitaille; 5; Andrew Thompson; 6; Karsten Kuhn; 6; Ian Pike; 6; Ryan Bomgarden; 2; John Rogers; 2; Steven Gygi; 1; Joao A. Paulo; 1; W.M. Fan; 2; Andrew N. Lane; 2; Laura S. Schmidt; 1; W. Marston Linehan; 1; 1; Yale University, New Haven; 2; University of Notre Dame, Notre Dame, IN

[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 W 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; University of Missouri-Kansas City, Kansas City, MO

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; 1; Yu Peng; 1; Lingjun Li; 1, 2; School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 2 Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222

Fructose Fluxomics of Fatty Acid Treated HepRG Cells to predict flux in NASH patients via LC-HRMS; Kyle Wald; 1; Anitha Saravanakumar; 2; Matthew Biatnik; 1; Fatemeh Akhlaghi; 2; Pfizer Inc., Groton, CT; 2; University of Rhode Island, South Kingstown, RI

Optimization of LC-MS/MS/MS conditions to improve the proteome coverage in 16-plex tandem mass tag-based proteomics; Shu Yang; 1; Mingming Niu; 1; Zhiping Wu; 1; Huan Sun; 1; Kaiwen Yu; 1; Danting Liu; 1; Junmin Peng; 1; St. Jude Children’s Research Hospital, Memphis, TN 38105

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; Thermo Fisher Scientific, San Jose, CA

Resolution of 13C and Deuterium Isotopes Allows High-Sensitivity Lipid Fluxomics Analysis Given Insight into Post-Prandial Lipid Metabolism; Matthew Mitsche; 1; Xiaorong Fu; 2; Jeffrey Mcdonald; 2; UTSW, Dallas; 2; University of Texas Southwestern Medical Center, Dallas, TX

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; 2; W. Marston Linehan; 2; National Institutes of Health, Bethesda, MD; 2; University of Kentucky, Lexington, KY

HRMS/MS-Based Approach for Separation and Quantification of Stable Isotope-Labeled Marfey’s Reagent Derivatized Physiological Amino Acids Stereoisomers; Nilish R. Mishra; 1; Amar Deep Sharma; 1; William G. Guthell; 1; University of Missouri-Kansas City, Kansas City, MO

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; Department of 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; Patrick Smyth\textsuperscript{1}; Xu Zhang\textsuperscript{1}; Zhibin Ning\textsuperscript{1}; Janice Mayne\textsuperscript{1}; Jasmin I Moore\textsuperscript{1}; Krystal Walker\textsuperscript{1}; Mathieu Lavallée-Adam\textsuperscript{1}; Daniel Figeys\textsuperscript{1}; \textsuperscript{1}University of Ottawa, Ottawa, ON
| WP 001 | The impact of mass spectrometry analysis on drug discovery of a human IgG2 bispecific antibody: Jia Dong1; Bryant Chau1; Feng Wang1; Gavin Dollinger1; Pavel Strop1; Arvind Rajpal1; 1Bristol-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 Jia1; Olivier Jean-Baptiste Mozziconacci1; 1MRL Analytical Sciences, Merck & Co. Inc., Rahway, NJ |
| WP 003 | Sensitive drug distribution measurements of an ADC with non-denaturing capillary SEC: Guillaume Tremintin1; Yue Ju1; Pan Mao2; Melvin A. Park3; 1Bruker, San Jose, CA; 2Newomics, Berkeley, CA; 3Bruker Daltonics, Billerica, MA |
| WP 004 | Mass Spectrometric Characterization of Antibody-siRNA Conjugate using the Agilent 6545XT AdvanceBio LC/Q-TOF: David Wong1; Balu Palani2; 1Agilent Technologies, Inc., Santa Clara, CA; 2Avidity Biosciences, Inc., La Jolla, CA |
| WP 005 | Evaluating the Sensitivity of the Synapt XS Mass Spectrometer for Analysis of Intact Monoclonal Antibody: Malcolm Anderson1; Lucy Fernandes2; Heidi Gastall2; Laetitia Denbigh2; Joanne Ballantyne3; 1WATERS, Cheshire, United Kingdom; 2Waters Corporation, Wilmslow, United Kingdom; 3Waters Corps, Milford, MA |
| WP 006 | Comparative Analysis of Glycopeptides between Biosimilars and Biosimilar of Infliximab by LC-ESI-MS/MS: Hyejin Kim1, 2; Geul Bang1; Myung Jin Oh2; Hyun Joo An2; Jin Young Kim1; Heeyoun Hwang1; Jong Shin Yoo1, 2; 1Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; 2Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea |
| WP 007 | A novel peptide-based quantification strategy to identify biomarkers from LFQ-based quantitative-proteomics data: Deeptarup Biswas1; Chetanya Gupta1; Sanjeeva Srivastava2; 1IIT Bombay, Mumbai, India; 2IIT Bombay, Mumbai, India |
| WP 008 | Mapping a Conformational Epitope of Hemagglutinin A Using Native MS and Ultraviolet Photodissociation: M. Rachel Mehaffey1; Keith R. Morgenstern1; Jiwon Lee1; Jiwon Jung1; Michael B. Lanzillotti1; Edwin E. Escobar1; George Georgiou1; Jennifer S. Brodbelt1; 1University 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. Kellie1; Nicole A. Schneck1; Matthew E. Szapacs1; 1GSK, Collegeville, PA |
| WP 010 | Middle-down Antibody Characterization Using ExD-based Fragmentation in a Q-TOF: Joseph C. Meeuwsen1, 2; Michael C. Hare1; Diana M. Oppenheimer1; Valery G. Voinov1, 2; Joseph S. Beckman1, 2; 1e-MSion, Inc., Corvallis, OR; 2Oregon 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 Bang1, 2; Hyejin Kim1; Myung Jin Oh2; Hyun Joo An3; Heeyoun Hwang1; 1Korea Basic Science Institute, Ochang, Cheongju-si, South Korea; 2College of Pharmacy, Korea University, Jochiwon, South Korea; 3Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea |
| WP 012 | A versatile method for quantitation of methionine oxidation in Fc fragment of therapeutic monoclonal antibodies using stable-isotope labelled internal standards: Tomasz K Godziewicz; Polpharma Biologics, Gdansk, Poland |
| WP 013 | Advancing mAb characterization with microchip CE-MS coupled to a PASEF enabled QTOF: J. Scott Mellors1; Guillaume Tremintin2; Scott B Fararo3, 4; Jarrod A Marto2, 4; 1908 Devices, Inc., Carrboro, NC; 2Bruker Scientific, San Jose, CA; 3Departments of Cancer Biology and Oncology Pathology, Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA; 4Departments 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 Xie1; Valerie Quarmby2; Jihong Yang2; 1Genentech, South SF, CA; 2Genentech 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 Jianan1; Zhou Yue2; Bo Tao3; 1ThermoFisher, Beijing, China; 2ThermoFisher Scientific, Shanghai, China |
**ART, ARCHAEOLOGY & PALEONTOLOGY**

**WP 016**

**Mass Spectrometric Identification of Collagen Preserved in Paleolithic Animal Remains;** Takashi Nakazawa¹; Momoko Osawa²; Mako Inuzuka¹; Kazuki Kawahara³; Seiji Kadowaki⁴; Yoshihiro Nishiaki⁵; 'Nara Women's University, Nara, Japan; ²Nagoya University, Nagoya, Japan; ³Osaka University, Suita, Japan; ⁴University of Tokyo, Bunkyo-ku, Japan

**WP 017**

**Organic compounds in the textile bandage of the Egyptian mummy; Olga Polyakova¹; Viatcheslav Artaev²; Olga Vasilyeva³; Maria Mednikova³; Jenya Anokhina⁴; Albert T Lebedev⁵; 'Moscow State University, Moscow, Russia; ²Rhein Main University, Ruesselsheim, Germany; ³University Of Liverpool, Liverpool, United Kingdom; ⁴Institute, Smithsonian Institution, Washington, DC**

**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 Anderson¹; Brian Thomas²; Lucien Tuinstra²; Stephania Herodotou³; Peter Myers³; Stephen Taylor³; 'Arizona Christian University, Glendale, AZ 85306; ²University 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-Martin¹; John George²; Emily Kaplan³; Lauren Osmond⁴; Leah Bright⁵; G. Asher Newsome⁶; Gwenaëlle Kavich⁷; Rachel Kaczkowski⁸; Susan Heald⁹; ¹Museum Conservation Institute, Smithsonian Institution, Suitland, MD; ²The National Museum of the American Indian, Smithsonian Institution, Washington, DC

**BIG ION MS**

**WP 021**

**Characterization of macromolecular complexes using multistage ultraviolet photodissociation mass spectrometry;** Ines C Santos¹; Jada N. Walker¹; Jennifer S. Brodbelt¹; '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 Jiang¹; Liam Dugan¹; Arezoo Shahvivarkevishahi²; Jeremiah J. Gassensmith³; Mark E. Bier¹; 'Carnegie Mellon University, Pittsburgh, PA; ²University of Texas at Dallas, Richardson, TX

**BIMARKERS: DISCOVERY II**

**WP 025**

**Quantitative Top-Down Proteomics of Tear Proteome Changes Related to Age;** Mick Greer¹; Daniel Lopez-Ferrer²; Romain Huguet²; Peter Verhaert³; Greg Foster⁴; Vad Zabrouskov⁵; Andreas Huhmer⁶; Peter Raus⁷; Ken Durbin⁸; Joe Greer⁹; Ryan Fellers¹⁰; Rich Leduc¹¹; 'Thermo Fisher Scientific, Austin, TX

**WP 026**

**DNA Aptamer Epitope Analysis as Antibody Alternatives Opens New Approaches for Biomarker Elucidation and Molecular Diagnostics;** Michael Przybylski¹; Loredana Lupu¹; Pascal Wiegand¹; Nico Huettmann¹;²; Stephan Rawer¹; Wolfgang Kleinekoford¹;²; Alexander Lazarrev³; Maxim Berezovski²; 'Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spec, Russelsheim, Germany; ²University of Ottawa, Ottawa, ON; ³Rhein Main University, Russelsheim, Germany; ⁴Pressure Biosciences Inc., South Easton, MA

**WP 027**

**Detailed characterization of aged human brain gangliosidose by high resolution multistage mass spectrometry;** Raluca Ica¹; Alina Petrut¹; Mirela Sarbu¹; Zeljka Vukelić⁴; Alina D. Zamfir⁵; 'National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; ²National Institute for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania, TIMISOARA, Romania; ³Department 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 Zhu¹; Junfeng Huang¹; Jie Zhang¹; Zhengwei Chen²; Yu Lin¹; Gabriela Grigorean¹; Lingjun Li³; Suyu Liu³; Amit G. Singal⁴; Neehar D. Parikh°; David M. Lubman¹; 'University of Michigan, Ann Arbor, MI; ²University of Wisconsin-Madison, Madison, WI; ³UT MD Anderson Cancer Center, Houston, TX; ⁴University 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 Maan¹; Ruchi Baghel¹; Radhika Bakhshi¹; Poonam Rana°; 'Institute of Nuclear Medicine & Allied Sciences (INMAS) - DRDO, Delhi, India; ²Institute of Nuclear Medicine & Allied Sciences (INMAS) - DRDO, Delhi, India; ³Shaheed 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 Nairn¹; Michael Wuczkowski²; Jesús Jiménez³; Iris Prinz⁴; Marco Rissoglio³; Emanuele Barborini⁵;²; Gerald Stübig⁶;³; 'Shimadzu, Manchester, UK, Manchester, United Kingdom; ²Medical University of Vienna,
**BIOMARKERS: QUANTITATIVE ANALYSIS II**

**WP 032** Metabolite and Lipid Profiling in Human Serum Related to Rheumatoid Arthritis; Yan-Ping Lin1; Wei-xuan Chen2; Rong Meng3; Gary W. Caldwell4; Wensheng Lang1; 1Janssen R&D LLC., Spring House, PA; 2Janssen 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 Lin1; Jianhui Zhu2; Jie Zhang3; Zhijing Tan1; Lingyuan Pan1; David M Lubman1; 1University of Michigan, Ann Arbor, MI

**WP 034** Comprehensive proteomic profiling of stool from IBD patients reveals biomarkers of disease activity; Brandon Harder1; Annemarie N Lekkerkerker1; Ellen P Casavant2; Marco Prunotto3; Jacqueline M McBride3; W Rodney Mathews4; Veronica G Anania4; 1Genentech Inc., South San Francisco, CA

**WP 035** An Ultra High-throughput Plasma Protein Profiling (uHTPP) Workflow Using a Modified Quadrupole-Orbitrap Mass Spectrometer; Michelle Dubuke1; Sarah Trusiak1; Ryan D. Bomgarden2; Sergei Snovida3; Bhavin Patel4; Emily Chen5; 1Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; 2Thermo Fisher Scientific, Rockford, IL; 3Thermofisher Scientific Precision Medicine Science Center, Cambridge, MA

**WP 036** Measurement of serum LPAs as potential biomarkers for COPD disease; Qingli Li1; Wei Tew2; Andrew Birnberg3; Arindam Chakrabarti4; Erik Verschuuren1; Carrie Rosenberger1; Michele Grimbaldeston1; Wendy Sandoval1; 1Genentech 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; Henrikos Dansses Seckler1; John T. Wilkins2; Jonathan Scott Rink3; Luca Forcelli4; Richard D Leduc1; Ryan T Fellers1; C Shad Thaxton5; Allan Sniderman4; Donald M Lloyd-jones2; Philip D. Compton5; Neil L Kelleher1; 1University of Nebraska Medical Center, Omaha, NE; 2Intercollegiate Faculty of Biotechnology University of Gdansk and Medical University of Gdansk, Gdansk, Poland; 3Clover Bioanalytical Software, Granda, Spain; 4Stratec Consumables, Salzburg, Austria; 5Tethis, Milan, Italy; 6Luxembourg Institute of Science and Technology, Beluva, Luxembourg; 7Comprehensive Cancer Center, Vienna, Austria

**WP 040** Utilizing Erythrocytes as Sources of Biomarkers for Alzheimer’s Disease; Jericha Mill1; Vihari Patel2; Tyler Ulland3; M. S. Salamat4; Ozioma Okonkwo5; Thomas Raife6; Lingjun Li1, 4; 1Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; 2Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; 3Clinical Science Center, Wisconsin Alzheimer’s Disease Research Center, University of Wisconsin School of Medicine and Public Health, Madison, Wisconsin; 4School of Pharmacy, University of Wisconsin-Madison, Madison, WI

**WP 041** Integrative discovery approach to identification of biomarkers in Fabry disease patient biofluids; Lisa A Crawford1; Maria Stella Ritorto1; 1Sanofi, Framingham, MA

**WP 042** Global Analysis of Protein Folding Stability Changes in a Mouse Model of Parkinson’s Disease; Michael C. Fitzgerald1; Renze Ma1; Julia Johnson1; 1Duke University, Durham, NC; 2Washington University in St. Louis, St. Louis, Missouri

**WP 043** Mass Spectrometry-Based Proteogenomics Analysis of Serum EGFR Family Proteins in Patients with Solid Tumors; Yun Chen1; Yuanyuan Zhang2; 1Nanjing Medical University, Nanjing, China

**WP 044** A Novel Derivationization Procedure for the Chemicals with Carboxylic Acid and Its Application in LC-MS/MS Bioanalysis; Dawei Zhou1; Yajie Zhang1; Sharon Tong1; 1WuXi AppTec, Cranbury, NJ

**WP 045** UPLC-MS/MS-Based Plasma Assay for Therapeutic Monitoring in Patients with APRT Deficiency; Unnur A. Thorsteinsdottir1; Hrafnhildur L. Runolfsdottir1; Finnur F. Eiriksson2; Vidar O. Edvardsson3; Runolfur Palsson1, 3; Margaret Thorsteinsdottir1, 2; 1University of Iceland, Reykjavik, Iceland; 2ArcticMass, Reykjavik, Iceland; 3Comprehensive proteomic profiling of stool from IBD patients reveals biomarkers of disease activity; Brandon Harder1; Annemarie N Lekkerkerker1; Ellen P Casavant2; Marco Prunotto3; Jacqueline M McBride3; W Rodney Mathews4; Veronica G Anania4; 1Genentech Inc., South San Francisco, CA

**WP 046** A comprehensive LC-MSMS method to quantitate key retinoids of the visual cycle; Mark Zambrowski1; Chung-Yeh Wu1; Siyuuan Shen1; Yubin Qiu1; Jennifer Campbell1; Christopher Adams1; Dennis Rice1; 1Novartis Institutes for Biomedical, Cambridge, MA

**WP 047** Targeted Method Package for Amino acid, Vitamins and Nucleotide Cell Culture Components; Xiaoxia Wang1; Yi Liu1; Zhengwei Jia1; 1Waters Technologies (Shanghai) Co, Ltd, Shanghai, China

**WP 048** A Multiple Reaction Monitoring (MRM) Approach to Investigate Macrophage Proteome; Katarzyna Macur1, 2; Andrew Schissel1; Sarah Zieschang1; Emma Harwood1; Brenda Morsey1; Howard Fox1; Pawel Ciborowski1; 1University of Nebraska Medical Center, Omaha, NE; 2Intercollegiate Faculty of Biotechnology University of Gdansk and Medical University of Gdansk, Gdansk, Poland

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**WEDNESDAY POSTERS (WP) Pages 86-124 | All posters will be on-demand content in the mobile app and online planner.**

Short abstract, Poster PDF, and optional presentation video will be included.
A Validated LC-MS/MS Assay for the Quantitation of 2-HG in Human Plasma Using A Surrogate Analyte Approach; Feng Yin; Yonghua Ling; Rohini Narayanaswamy; Heidi Mangus; Fumin Li; Hua Yang; Guowen Liu; 1Agios Pharmaceuticals, Inc., Cambridge, MA; 2PPD, Middleton, WI

High Throughput Quantitation of Human Milk Oligosaccharides in Breast Milk Samples Yields Variation from Geographically Diverse Sites; Anita Vinjamuri; Jasmine Davis; Juan J. Castillo; Carlito B Lebrilla; 1UC Davis, Davis, CA

Increasing the Ease of Use and Robustness of Nanoflow with Plug and Play Low Flow Source; Arianna I Jones; Christie Hunter; Thomas Vander Schans; Saghar Kaabinejad; Ken Jackson; Curtis Mcmurtrey; 1SCIEX, Framingham, MA; 2SCIEX, Redwood Shores, California, 1201; 3Pure MHC, Oklahoma City, OK

Global & targeted proteomic analysis reveals the presence of distinct proteomic signatures associated with Skull base vs Supratentorial meningiomas; Shuvolina Mukherjee; Deeptarup Biswas; Aliasgar Moiyadi; Sridhar Epari; Sanjeeva Srivastava; 1Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, India; 2Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, Maharashtra, India, Mumbai, India; 3Department of Pathology, Tata Memorial Centre, Mumbai, Dr. E Borges Road, Parel, Mumbai, India

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; Wen Tang; Yves Sabbagh; Bailin Zhang; 1Sanofi Genzyme, Framingham, MA

Urinary Proteomics Reveals Putative Biomarkers Associated with Renal Function in Pediatric Patients with Ureteropelvic Junction Obstruction; Dijana Vitko; Shannon E. DiMartino; Tanya Logvinenko; Hsin-Hsiao Wang; John W. Froehlich; Richard S. Lee; 1Boston Children's Hospital, Boston

A mass spectrometry-based approach for quantifying low-level products of prohormone processing in human plasma; Yinyin Ye; Adam C. Swensen; Yuqian Gao; Thomas Fillmore; Tujiun Shi; Wei-Jun Qian; 1Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington

Efficient Separation and Identification of 33-mer Gliadin Peptide and its Various Deamidated Forms Using Ultra-high-resolution LC/MS; Jie Pu; Chao Xue; Matthew Szapacs; Thomas Angel; Jun Qu; 1SUNY at Buffalo, Buffalo, NY; 2GSK, Collegeville, PA

Multi-Omic Biomarkers of Cellular Senescence; Nathan Basisty; Abhijit Kale; Chisaka Kuehnenmann; Samah Shah; Toshiko Tanaka; Vagisha Sharma; Luigi Ferrucci; Judith Campisi; 4; Birgit Schilling; 1The Buck Institute for Research on Aging, Novato, CA; 2Intramural Research Program of the National Institute on Aging, NIH, Baltimore, Maryland; 3University of Washington, Seattle, WA; 4Lawrence Berkeley Laboratory, University of California, Berkeley, California

Deeper Kinome Coverage Using Multi-inhibitor Enrichment and Trapped Ion Mobility Mass Spectrometry; Robert Sprung; Petra Erdmann-Gilmore; Michael East; Gary L Johnson; R Reid Townsend; 1Washington University School of Medicine, St. Louis, MO; 2University of North Carolina at Chapel Hill, Chapel Hill, NC

Comparing whole blood lysates to Dried Blood Spots in targeted LC-MS/MS Proteomic Methods to detect markers of autologous blood transfusion; Matt Kuruc; Swapan Roy; Johan Jakobsson; Raik Wagner; Christer Malm; 1Biotech Support Group LLC, Monmouth Junction, NJ; 2Pro Test Diagnostics AB, Umeå, Sweden

In-gel cross-linking mass spectrometry (IGX-MS) benefits the analysis of distinctive protein complexes in selectivity and sensitivity; Marie V. Lukassen; Johannes F. Heveler; Albert J.R. Heck; 1Biomolecular Mass Spectrometry and Proteomics, Utrecht Institute for pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands

Investigation of Noncovalent Interactions Between Peptides with Potential Intrinsic Sequence Patterns by Mass Spectrometry; Chuan-Fan Ding; Shulong Yang; Qi Guo; Fangling Wu; Yuhong Wang; 1Ningbo University, Ningbo, China; 2Fudan University, Shanghai, China

Systematic evaluation of amphiphilic structure environments on protein modification by fast photochemical oxidation of proteins; Zhi Cheng; Joshua Sharp; 1University of Mississippi, Oxford, MS

Fast and highly efficient affinity enrichment of Azide-A-DSBSO cross-linked peptides from a complex matrix; Manuel Matzinger; Wolfgang Kandioller; Philipp Doppler; Elke Heiss; Karl Mechtler; 1Institute of Molecular Pathology (IMP), Vienna BioCenter (VBC), Vienna, Austria; 2Institute of Inorganic Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; 3Institute of Chemical, Environmental and Bioscience Engineering, Vienna University of Technology, Vienna, Austria; 4Department of Pharmacognosy, Faculty of Life Sciences, University of Vienna, Vienna, Austria; 5Institute 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\(^1,2\); Alan G. Marshall\(^2,3\); Shana V. Stoddard\(^1\); Joshua S. Sharpe\(^1\); 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 Martinez\(^1\); 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\(^2,3\); 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\(^2,3\); Yuxin An\(^1,2,3\); Lili Zhao\(^2,3\); Hang Gao\(^1,2,3\); 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 Kolbowksi\(^1\); Martin Graham\(^2\); Juri Rappisiber\(^1\); \(^1\)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\(^1\); Trisha N. Davis\(^1\); 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\(^3\); Diogo Borges Lima\(^1\); Fabio Cesar Gozzo\(^2\); 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); Savan Gupta\(^1\); Matthew Rosi\(^2\); Brandon Russell\(^2\); Shawn Costello\(^2\); 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, Menlo Park, California
Performance of serum apolipoprotein E measurement in EQA program with targets by isotope dilution LC-MS/MS; Qing Li1; Yi Ju1; Zhonggan Jin1; Hewei Sun1; 1shanghai center for clinical laboratory, shanghai, China

A High-Resolution Liquid Chromatography-Mass Spectrometry Method for Identification of Toxic Natural Products in Clinical Cases; Y. Ruben Luo1; Robert Goodnow2; Kate Costomck3; Cassandra Yun1; Kara L Lynch1; 1University of California San Francisco, San Francisco, CA; 2Baylor College of Medicine, Houston, TX; 3Thermo Fisher Scientific, San Jose, CA

Matrix effects-free determination of fentanyl in biological samples with Bio-SPME using a modified microfluidic open interface coupled to LEI-MSMS; Priscilla Rocio Bautista1; Giorgio Famigli2; Veronica Termopoli3; Pierangela Palma4, 3; Emir Nazdrajić4; Janusz Pawliszyn5; Achille Cappiello2, 3; 1University of Parma, Parma, Italy; 2University of Urbino, Urbino, Italy; 3Vancouver Island University, Nananimo, BC; 4University of Waterloo, Waterloo, ON

HPLC-MS/MS determination of cyclosporine A concentrations in pediatric patients undergoing HSCT and the relationship between cyclosporin; Ziyi Yang1; Lei Wang1; Jianping Zhang1; Ying Zhao2; Hongxing Liu1, 3, 4; 1HebeiYandu Daopei Hospital, Langfang, China, China; 2Hebei Yandu Lu Daopei Hospital, Langfang, China, China; 3Beijing Lu Daopei Institute of Hematology, Beijing, China; 4Beijing Lu Daopei Hospital, Beijing, China

Quantitative Urinalysis for Drugs of Abuse and their Metabolites using Paper Spray Mass Spectrometry (PS-MS) for Clinical and Forensic Toxicology; Scott A. Borden1, 2; Armin Saatchi1; Jan Palaty2; Erik T. Krogh1, 2; Christopher G. Gill1, 2, 4, 5; 1Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC; 2University of Victoria, Victoria, British Columbia; 3Lifelabs Medical Laboratories, Burnaby, BC; 4Simon Fraser University, Burnaby, BC; 5University of Washington, Seattle, WA

Optimization Using LC-MS/MS; Hsin Ho1; David Marchisin1; Huidong Gu1; Todd Lusk2; Raj Mangaraj3; Wenying Li1; John Brailsford1; Anjaneya Chimalkonda1; Jim Shen1; 1Bristol-Myers Squibb, Princeton, NJ; 2Q2 Solutions, Ithaca, NY

An Innovative Approach to Absolute Bioavailability Assessment with Strategic Isotopic labelling Optimization and Quantitation of Antibiotics in Dried Plasma Spots Utilizing Paper Spray Mass Spectrometry; Christine Skaggs1; Nicholas Manicke1, 2; Neloni Wijeratne3; Lindsey Kirkpatrick3; 1Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 2Forensics and Investigative Sciences, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 3Thermo Fisher Scientific, San Jose, CA; 4Department of Pediatrics, Division of Pediatric Infectious Diseases, Indiana University School of Medicine, Indianapolis, IN

Optimization of Antibiotics in Dried Plasma Spots Utilizing Paper Spray Mass Spectrometry; Christine Skaggs1; Nicholas Manicke1, 2; Neloni Wijeratne3; Lindsey Kirkpatrick3; 1Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 2Forensics and Investigative Sciences, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 3Thermo Fisher Scientific, San Jose, CA; 4Department of Pediatrics, Division of Pediatric Infectious Diseases, Indiana University School of Medicine, Indianapolis, IN

LC-MS/MS Analysis of Statram Corneum on Skin Tape Strips – Current Development Towards Diagnostics of Endotypes of Atopic Diseases; Evgeny Berdyshyev1; Irina Bronova1; Elena Goleva1; Donald YM Leung1; 1National Jewish Health, Denver, CO

Probe ElectroSpray ionization for breast cancer rapid identification; Enrico Davoli1; Silvia Giordano2; Hidekazu Saiki3; Takaaki Hiraoka4; Rita De Sanctis5; Rosalba Torrisi5; Daniela Pistillo5; 1Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; 2Shimadzu Italia SRL, Milan, Italy; 3Shimadzu Corporation, Kyoto, Japan; 4Shimadzu Europa GmbH, Duisburg, Germany; 5Humanitas Clinical and Research Center – IRCCS, Milano, Italy

Towards a point-of-care method to quantify tenofovir diprophosphate in human whole blood for adherence monitoring; Sangeeta Pandey1; Fan Pu1; Lane R. Bushman2; Peter L. Anderson2; Zheng Ouyang1, 3; R. Graham Cooks1; 1Department of Chemistry, Purdue University, West Lafayette, IN; 2Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado Denver, Aurora, CO 80045; 3Department of Precision Instrument, Tsinghua University, Beijing, China

Multiplex quantification of immunomodulatory proteins in tissue and plasma using targeted MRMAss spectrometry; Jeff Whiteaker1; Lei Zhao1; Jacob Kennedy1; Regine Schoenherr1; Richard Ivey1; Julia Voytovich1; Amanda G Paulovich1; 1Fred Hutchinson Cancer Research Center, Seattle, WA

Protective mechanism of dried blood spheroids; Benji Frey1; Deidre E. Damon1; Danyelle M. Allen1; Jill Baker1; Sam Asamoah1; Abraham K. Badu-Tawiah1; 1The Ohio State University, Columbus, OH

A comprehensive label-free proteomic profiling of medulloblastoma Group-3 tumors; Manubhai Kp1; Anurag Kumar1; Deeptarup Biswas1; Epari Sridhar2; Aliasgar Moiyadi2; Neelam Shirsat3; Sanjeeva Srivastava1; 1IIT Bombay, Mumbai, India; 2Tata Memorial Center (Hospital), Mumbai, India; 3ACTREC, Mumbai, India
**WEDNESDAY POSTERS (WP) Pages 86-124 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.**

**WP 101**
An antibody-free LC-MS/MS method for the quantification of intact IGF-1 and IGF-2; Mark S Pratt1; Martijn Van Faassen1; Noah Rammels1; Rainer Bischoff2; Ido P Kema1; 1Department of Laboratory Medicine, University Medical Center Groningen, University of Groningen, Groningen, Netherlands; 2Analytical 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 Gao1; Fangfei Zhang1; Shuang Liang1; Qiushi Zhang1; Yi Zhu1; Tianran Guo1; 1Westlake University, Hangzhou, China

**WP 103**
Human Histones Characterization using LC-TIMS-TOF MS; Thao Ngoc Pham1; Cesar E. Ramirez2; Yasir Mamun3; Francisco Alberto Fernandez-Lima1; 1Florida International University, Miami, FL

**WP 104**
Analysis of dexamethasone and 6-OH dexamethasone in rabbit plasma, aqueous and vitreous humors, and retina by UHPLC-MS/MS; Jianghong Gu1; Jiang Wang1; Ashok Chockalingam1; Lin Xu1; Sharron Stewart1; Yan Wang1; Patrick Faustino1; Dian Shakleya1; 1FDA, Silver Spring, MD

**WP 105**
In vivo Proximity Labeling for Cell-type Specific Proteomics; Sydney N Sunna1; Sruti Rayaprolu1; Ranjita Betarbet1; Hailian Xiao1; Lihong Cheng1; Allan Levey1; Nicholas T Seyfried1; Srikant Rangaraju1; 1Emory 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 Badal1; Marta Sans2; Sanghoon Lee3; Sara Corvigno4; John Lin5; Michael Keating6, 7; Jingsong Liu8; Anil Sood9; Livia Eberlin10; 1University of Texas at Austin, Austin, TX; 2University of Texas at Austin, Austin, Texas; 3The University of Texas MD Anderson Cancer Center, Houston, TX; 4University of Texas, 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 Sun1; Daniela Konforty1; Dawn-Marie Murphy McLean1; Jan Palaty2; 1Lifelabs Medical Laboratories, Toronto, ON; 2Lifelabs Medical Laboratories, Burnaby, BC

**WP 108**
Tumorous cell percentage determination by ambient molecular profiling of gliomas; Stasios Pekov1, 2; Denis Bormotov1, 2; Anuradha Shripak1; Vasily Eliferov1; Vsevolod Shurkhay1, 2; Alexander Potapov1; Eugene Nikolaev1, 2; Anatoly Sorokin1; Igor Popov1, 2; 1Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 2V.L. Tarase Institute for Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; 38. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; 4Skolkovo 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 Xu1; Brian Slay1; Nikolina Babic1; 1Department of Pathology and Laboratory Medicine, Medical University of South Carolina, Charleston, South Carolina

**CORPORATE POSTERS III**

**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**
A new method for improving LC-TOF/MS detection limits using simultaneous ion counting and waveform averaging; Yousuke Kawai1; Yumi Miyake2; Toshinobu Hondo3, 4; Jean-Luc Lehmann4; Kentaro Terada1, 2; Michisato Toyoda2; 1Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Japan; 2Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Toyonaka, Japan; 3MS-Cheminformatics, Inabe-gun, Japan; 4Acqiris SA, Geneva, Switzerland

**WP 115**
Applications of Ti4 as a Diagnostic Reagent for the Detection of Sulfoxide-containing Metabolites or Impurities of Pharmaceuticals using UHPLC-MS/MS; Li-Kang Zhang1; Ping Chen1; Hong Li1; Douglas Richardson1; 1Merck Research Laboratories, Kenilworth, NJ

**WP 116**
Determination of N-nitrosodimethylamine in metformin hydrochloride sustained-release tablets by LC-MS / MS; Yong Wang; shimadzu(china) CO.,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 Liu1; Da Chen1; Niusheng Xu1; 1Thermo Fisher Scientific, Shanghai, China
Predicting the Future - Heading off Bioanalytical Issues with Two Solutions for Small Molecule In Vivo Quantitation; Rachael K Bridgman; AbbVie, North Chicago, IL

High Resolution LC/MS Database Search Capability Across Multiple LC/MS Vendor Platforms Using a Custom Interface Program; Michael P Mawn1; Jeff Gilbert2; Chris Brown2; Yelena Adelfinskaya2; Jeffrie Godbey2; Jesse Balcer2; 1Corteva Agriscience, Newark, DE; 2Corteva Agriscience, Indianapolis, IN

LC-APCI-dMRM Method for Quantification of Eight Nitrosamine Impurities in ARB Drugs; Raghavi Kakarla1; Tim Andres Marzan1; Jingyue Yang1; 1FDA, Saint Louis, MO

Development of Rapid Analytical Screening Methods by Thermal Desorption-Electrospray ionization/Mass Spectrometry (TD-ESI/MS) for Novel Oral Anticoagulants (NOACs); Yu-Ming Hsu1; Tzu-Yu Pan1; Chia-Fang Wu1; Ming-Tsang Wu1, 2, 3, 4; 1Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; 2Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung, Taiwan; 3Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan; 4Ph.D Program of Environmental and Occupational Medicine and Graduate Institute of Clinical Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan

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 Pan1; Sih-Syuan Li1; Yu-Ming Hsu1; Ming-Tsang Wu1, 2, 3, 4; Chia-Fang Wu1; 1Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; 2Ph.D Program in Environmental and Occupational Medicine, Kaohsiung Medical University, Taiwan; 3Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan; 4Graduate Institute of Clinical Medicine, Kaohsiung Medical University, Taiwan; 5Department of Community Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Taiwan

Simultaneous quantitation of dexamethasone and dexamethasone phosphate in mice plasma and organ tissue by triple quadrupole LC-MS/MS with isotope dilution; Michelle L Spruill1; Howard Martin2; Xinli Liu1; 1University of Houston College of Pharmacy, Houston, TX; 2Sagis Diagnostics, Houston, TX

Hydrogen/Deuterium and 16O/18O exchange mass spectrometry can boost the reliability of the compound identification; Yury Kostyukevich1; Oxana Kovalova1; Alexander Zherebker1; Eugene (evgeny) Nikolaev2; 1Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; 2Skolkovo institute of science and technology, Moscow Region, Russian Federation

Routine, ultra-trace analysis of nitrosamines in drugs using Gas Chromatography – Orbitrap Mass Spectrometry; Dominic Roberts1; Giulia Riccardino2; Cristiano Cojocariu2; Aaron Lamb2; Jason Cole3; 1Thermo Fisher Scientific, Runcorn, United Kingdom; 2Thermo Fisher Scientific, Runcorn, United Kingdom; 3Thermo Fisher Scientific, Austin, TX

UV-Photodissociation on a hybrid QqLIT mass spectrometer to increase selectivity in LC Analysis; Yves Le Blanc1; Mircea Guna2; Jeff Gilbert3; 1SCIEX, Concord, On, ON; 2SCIEX, Concord, ontario; 3Corteva Agriscience, Indianapolis, IN

Unraveling the Gut Microbiome’s Direct and Indirect Effects on Human Drug Metabolism; Alan K. Jarmusch1; Alison Urbana2; Jeremiah D. Momper2; Joseph D. Ma3; Maher Alhaja3; Marlion Liyanage3; Rob Knight3, 4, 5; Shirley M. Tsunoda3; Pieter C. Dorrestein1, 2, 4; 1Skaggs School of Pharmacy and Pharmaceutical Sciences and Collaborative Mass Spectrometry Innovation Center, University of California, San Diego, La Jolla, CA; 2Department of Pediatrics, University of California, San Diego, La Jolla, CA; 3Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA; 4Center for Microbiome Innovation, University of California San Diego, La Jolla, California; 5Department of Computer Science and Engineering, University of California, San Diego, La Jolla, CA

Equine in vivo metabolites of the selective androgen receptor modulators (SARMs) LGD-3033 and ACP-105 determined using high-resolution mass spectrometry; Malin Nilsson Broberg1; Heather Knych2; Ulf Bondesson1; Curt Pettersson1; Börje Tidstedt3; Scott Stanley4; Mario Thevis5; Mikael Hedeland1, 3; 1Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden; 2Kenneth L. Maddy Equine Analytical Pharmacology Laboratory, School of Veterinary Medicine, University of California, Davis, CA; 3National Veterinary Institute (SVA), Uppsala, Sweden; 4University of Kentucky, Gluck Equine Research Center, Lexington, KY; 5German Sport University, Centre for Preventive Doping Research, Cologne, Germany

Structure identification of glyoxylate and cyanide reaction products by mass spectrometry; Xu Shi; Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA

In vitro AmpC-mediated hydrolysis of β-lactams and the rapid detection of downstream metabolites by LC-MS/MS; Anthony M. Haag1, 2; Thomas D. Horvath1, 2; Sigmund J. Haidacher1, 2; Kathleen M. Hoch1, 2; Jennifer K. Spinler1, 2; 1Baylor College of Medicine, Houston, TX; 2Texas Children’s Hospital - Microbiome Center, Houston, TX
WP 132 Pharmacokinetics of fluoxetine in horse; Charley Veitri1; Laura Waitt-Wolker2; Krista Pearman3; Maria Lozoya4; Jeffrey W. Norris5; 1Midwestern University College of Pharmacy-Glendale, Glendale, AZ; 2Midwestern University College of Veterinary Medicine, Glendale, AZ; 3Midwestern University College of Graduate Studies, Glendale, AZ

WP 133 An Automated Approach to Urine Sample Preparation Employing Room Temperature Enzymatic Hydrolysis; Jeremy Smith1; Jillian Neifeld1; Elena Girloch1; 1Biotage, LLC, Charlotte, NC

WP 134 Measuring relevant markers in the place they matter: metabolomics of cerebrospinal fluid for better pediatric brain tumor therapy; Boryana Petrowa; 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 Jiang1; Min Du2; Kate Comstock2; 1Amgen Inc., South San Francisco, CA; 2Thermo Fisher Scientific, San Jose, California

WP 136 Mass spectrometric investigation and theoretical modeling of triazole complexes with amino acids; Alisa Tokareva1; Vitaliy Chagovets2; Alexey Kononikhin1; Natalia Starodubitseva1; Vladimir Frankovich1; 1FSBI «National Medical Research Center for Obstetrics, Gynecology and Perinatology Named After Academician V.I.Kulakov» Ministry Of Healthcare of the Russian Federation, Moscow, Russia

WP 137 A Course Undergraduate Research Experience (CURE) Featuring Peptide Mass Spectrometry; Jay G Forsythe1; Michael W Giuliano1; 1College of Charleston, Charleston, SC

WP 138 Rapid Trypsin Digest for Peptide Analysis and Protein Identification in a Classroom Laboratory by MALDI-TOF; Matthew A Portis1; Alexander D. Jacobs1; 1University 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

WP 140 Analytical tools for the specciation analysis in biocrudes; Victor Garcia-Montoto1,2; Sylvain Verdier3; Jan H Christensen4; Brice Boyussiere1; 1University of Pau and Pays de l'Adour, CNRS, UMR5264, IPREM, Pau, France; 2University of Copenhagen, Frederiksberg, Denmark; 3Haldor Topsoe A/S, Lyngby, Denmark

WP 141 Inhibition of TOR in Chlamydomonas reinhardtii Leads to Rapid Cysteine Oxidation Reflecting Sustained Physiological Changes; Amanda L. Smythers1; Megan M. Ford1; Evan W. Mcconnell1; Sarah C. Lowery1; Derrick R.J. Kolling2; Leslie M. Hicks1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2Marshall University, Huntington, WV

WP 142 Distinguishing Routes of Gas-Phase Pyrolysis of Sulfonated Phenethyl Phenyil Ethers Using Collision-Induced Dissociation Mass Spectrometry; Cory J Conder1; Sabyasachy Mistry1; Paul G Wenthold1; 1Purdue University, West Lafayette, IN

WP 143 KairosMS: A solution for complex mixture data analysis and visualisation; Hugh E. Jones1; Remy Gavard1; Diana Catalina Palacio Lozano1; Mary J. Thomas1; Mark P. Barrow1; 1University of Warwick, Coventry, United Kingdom

WP 144 Energy-resolved MCAD of Seven Isomeric n-Pentylquinoline Radical Cations; Yuyang Zhang1; Haoran Lei1; Hilkka I. Kenttämaa1; 1Purdue University, West Lafayette, IN

WP 145 Characterization of hydrodeoxygenated bio-oils by Fourier transform ion cyclotron mass spectrometry; Kimi Kekäläinen1; Idoia Hita Del Olmo1; Tomás Cordero Lanzaci1; Giff Ogechukwu Okafor1; Pedro Castaño2; 1University of Eastern Finland, Joensuu, Finland; 2Multiscule Reaction Engineering, KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia; 3Department 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-Andrivet1,2; Clément Castilla1; Christopher P. Rüger1,3; Anna Luiza Mendes Siqueira2; Marie Hubert-Roux1; Carlos Afonso1; 1University of Rouen-Normandy, Mont-Saint-Aignan, France; 2Total, Marketing Services, Research Center, Solaize, France; 3University 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. Abraham1; Hannah K. Liberatore2; Michael J. Plewa3; Elizabeth D. Wagner4; Susan D. Richardson1; 1University of South Carolina, Columbia, SC; 2US Environmental Protection Agency, Raleigh, NC; 3University of Illinois at Urbana-Champaign, Urbana, IL
**ENVIRONMENTAL: EXPOSOMICS**

**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; Elena I. Panagopoulou; Adamantia Agaliou; Dimitris Beis; Carsten Baessmann; Artem Filipenko; Nikolaos S. Thomaidis; 1National and Kapodistrian University of Athens, Athens, Greece; 2Biomedical Research Foundation Academy of Athens, Athens, Greece; 3Bruker Daltonik GmbH, Bremen, Germany; 4Bruker 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; James N. Dodds; Molly T. Soper-Hopper; Markace Rainey; Facundo M. Fernandez; Erin S. Baker; 1Department of Chemistry, North Carolina State University, Raleigh, North Carolina; 2Department of Chemistry, Northern Kentucky University, Highland Heights, Kentucky; 3School 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; Juan A. Aristizabal-Henao; John A. Bowden; 1University of Florida, Gainesville, FL

**WP 152**  
Profiling Exposure-Dependent Protein Destabilization Through the Proxy of Hsp40 Affinity; Joseph Genereux; Guy Quanrud; Maureen R Montoya; 1University of California, Riverside, Riverside, CA; 2University 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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Development of DNA Adductome Mass Spectral Database; Jingshu Guo; Robert J. Turesky; Anamary Tarifa; Anthony P. De Caprio; Marcus S. Cooke; Scott J. Walmsley; 1University of Minnesota, Minneapolis, MN; 2Florida 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; Wilfred J. J. Kammaus; Su Chen; Susan Ewart; Syed Hasan Arshad; John W. Holloway; Hongmei Zhang; A. Daniel Jones; 1Michigan State University, East Lansing, MI; 2Division of Epidemiology, Biostatistics, and Environmental Health, School of Public Health, University of Memphis, Memphis, Tennessee; 3Department of Mathematical Sciences, University of Memphis, Memphis, Tennessee; 4Department of Large Animal Clinical Sciences, College of Veterinary Medicine, Michigan State University, East Lansing, Michigan; 5Clinical and Experimental Sciences, Faculty of Medicine, University of Southampton, Southampton, United Kingdom; 6The David Hide Asthma and Allergy Research Centre, Isle of Wight, United Kingdom; 7NIHR Respiratory Biomedical Research Unit, University Hospital Southampton, Southampton, United Kingdom; 8Human Development and Health, University of Southampton, Southampton, United Kingdom; 9Department 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; Rachel Koerber; Joann Lucero; Jake Mcdonald; Amie K. Lund; 1University of North Texas, Denton, TX; 2Lovelace Biomedical, Albuquerque, NM

**WP 157**  
Monitoring of exogenous compound kinetics in exhaled breath; Tanja Zivkovic Semren; Csaba Laszlo; Marta Gomez; Guillermo Vidal-de-Miguel; Julia Hoeng; Manuel Peitsch; Nikolai Ivanov; Philippe A. Guy; 1Philip Morris Products SA, Neuchatel, Switzerland; 2Fossil Ion Technology, Madrid, Spain

**WP 158**  
Repurposing Public Metabolomics Datasets for Construction of an Exposomics Spectral Library; Biswapriya Biswavas Misra; Independent Researcher, Namburu, India

**FOOD SAFETY: GENERAL I**

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Survey of Antibiotic Residues in Dried Distiller’s Grains with Solubles from 14 Different States by LCMS; Kevin R Tucker; Samantha A Olendorff; Karolina Chmielewska; 1Southern 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; Erasmus Cudjoe; 1PerkinElmer Inc., Woodbridge, ON; 2Perkin Elmer, Waltham, MA
WP 161 Rapid Quantitation of Veterinary Dyes in Salmon Extracts Using PaperSpray Coupled with a TSQ Altis MS; Neloni R Wijeratne1; Katherine Walker1; Ed George1; Laura E Burns2; Dwayne E Schrunk2; 1Thermo Fisher Scientific, San Jose, CA; 2Iowa State University, Ames, IA

WP 162 Real-Time Chemical Puff Profiling of ENDS Aerosol with Chemical Ionization - Mass Spectrometry; Alessandra Paul1; Devon O'regan1; Jeremy Nowak1; Luca Cappellin2; Nadja Heine1; 1JUUL Labs, San Francisco, CA; 2Tofwerk, 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 Ishioka1; Miho Kawashima2; Manami Kobayashi1; Junichi Masuda1; Yoshihiro Hayakawa1; 1Shimadzu Corporation, Hadano, Japan; 2Shimadzu 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 Kou1; Kiotaoka Konuma1; Kirk R. Jensen2; John Gonzales2; Kazuaki Murayama1; Yoshihisa Ueda1; 1JEOL Ltd, Akishima, Japan; 2JEOL 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 Serino1, 2; Yoshizumi Takigawa1; Takeshi Otsuka1; Sadao Nakamura1; Tarun Anumol1; Shigehiko Kanaya2; 1Agilent Technologies, Hachioji, Japan; 2Nara Institute of Science and Technology, Ikoma, Japan; 3Agilent Technologies, Wilmington, DE

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 Lupo1; Randy Ronesberg1; Xiaoning Lu1; 1Restek, Bellefonte, PA

WP 167 Determination of phthalate contamination onto plastic wrapped cucumbers using MALDI MS imaging; Phoebe Bray1; Catherine Duckett1; Robert Bradshaw1; 1BMRC, 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 Ghosh1; Amadeo Fernández-Alba2; Łukasz Rajski1; Charles T. Yang1; Olaf Scheibner2; Łukasz Rajski1; Christian Klaas3; 1Thermo Fisher Scientific, San Jose, CA; 2UNIVERSIDAD DE ALMERÍA, Almería, Spain; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

WP 170 Evaluation of food processing methods in removing pesticide residues in celery – LC/Q-TOF MS analysis; Yao Ling1; Ebony Kia Thornton1; 1SCSU, 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 Joseph1; Aimei Zou1; Limian Zhao2; Ruben Garnica2; Dan-Hui-Dorothy Yang3; Patrick Batoon1; Chee-Sian Gan1; 1Agilent Technologies Singapore (Sales) Pte Ltd, Singapore, Singapore; 2Agilent Technologies, Wilmington, DE; 3Agilent Technologies, Santa Clara, CA

WP 172 USB Powered Coated Blade Spray Ion Source for future on-site food testing by portable Mass Spectrometry; Marco Blokland1; Josha Jager1; Arjen Gerssen3; Janusz Pawliszyn2; Michel Nielen1,2; 1Wageningen University and Research, OTC, Wageningen, Netherlands; 2University of Waterloo, Waterloo, ON; 3Wageningen University and Research, OTC, Wageningen, Netherlands

WP 173 Development of LC-MS/MS method for determination of microbial trans-glutaminase in food; Irina Goncharova1; Zoya Nikiforova1; Elizaveta Goncharova1; Ilya Batov1; Denis Nekrasov1; Olga Ivanova1; Renat Selimov1; 1VGNKI, 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 Yang1; Guannan Li2; Tina Chambers2; 1Agilent Technologies, Inc, Santa Clara, CA; 2Agilent 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
WP 178  Examining Transfer Efficiency of Paper Substrates Utilized as Physical Transfer Swabs; Jessica M. Holtz; Trevor J. McDaniel; Alex Swiontek; Christopher C. Mulligan; Illinois State University, Normal, IL

WP 179  Development of an Updated Forensic DART-MS Mass Spectral Database; Edward Sisco; Arun Moorthy; National Institute of Standards and Technology, Gaithersburg, MD; National Institute of Standards and Technology, Gaithersburg, MD

WP 180  TIMS-qToF-MS for the investigation of electrochemically generated isomers of xenobiotics; Oxana Korzenko; Uwe Karst; University of Münster, Münster, Germany

WP 181  Identification of synthetic opioid analogs by high-resolution tandem mass spectrometry and machine learning; Xinyi Sui; Yufei Chen; Nelson Vinuela; North Carolina State University, Raleigh, NC

WP 182  Isobaric Drug Analyses Using Desorption Atmospheric Pressure Chemical Ionization and Online Derivatization; Christopher M. McDonald; Michael C Godwin; Edgar Torres; William Hoffmann; 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; Dong Zhang; Gerardo Gamez; Texas Tech University, Lubbock, TX; Texas Tech University, Lubbock, Texas

WP 184  Using DIA Analysis of Genetically Variant Peptides for Human Identification; Paul A Rudnick; Sanne Aalbers; Daniel Chelsky; Richard Johnson; Brian Searle; Bruce Weir; Michael J MacCoss; Spectragen Informatics, Bainbridge Island, WA; University of Washington, Seattle, WA; Institute for Systems Biology, Seattle, WA

WP 185  Protein-Based Body Fluid Identification: Specificity and Sensitivity; B. Mckay Allred; Glenn Kresge; Henry Zheng; 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; Katie-Jo Teehan; Lee Williams; Geoff Davies; Adam Senior; Alan Edgington; Helen Lodder; Jillian Neifeld; Biotech GB Limited, Cardiff, United Kingdom; Biotech, Charlotte, North Carolina

WP 187  Matching Forensic Proteome Profiles to Genetic Sequences through the Detection of Genetically Variable Peptides from Fingerprint Touch Samples; Myles W Gardner; F. Curtis Hewitt; Michael A. Freitas; August E. Woemer; Alan R. Smith; Andrew J. Reed; Danielle S. LeSassier; Maryam Baniasad; Katharina Weber; Leah W. Allen; Megan E. Powals; Benjamin C. Ludolph; Benjamin Crysup; Anthony D. Kappell; Signature Science, LLC, Austin, TX; The Ohio State University, Columbus, OH; 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; Meghan C. Burke; William E. Wallace; Yuxue Liang; Sergey Sheetlin; Yuri A. Mirokhin; Dmitrii V. Tchekhovskoi; Stephen E. Stein; 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; Robert H Powers; Alyssa L M Marsico; University of New Haven, West Haven, CT

WP 190  Analysis of Synthetic Cannabinoids in Plant Materials Using a LDTD-MS/MS System; Sandra Imrazene; Serge Auger; Jean Lacoursière; Pierre Picard; Phytronix Technologies, Quebec, QC

WP 191  Identification and Quantification of Metoprolol in Equine Plasma by LC-MS/MS; Jaclyn R. Missanelli; Youwen You; Rachel M. Proctor; Mary A. Robinson; University of Pennsylvania, Kennett Square, PA; PA Equine Toxicology and Research Laboratory, West Chester, PA

WP 192  Fingermark Sampling Using Particle Capture Mass Analysis with Nanoparticles; Jamira Stephenson; Kermit K Murray; Louisiana State University, Baton Rouge, LA

FUNDAMENTALS: ION SPECTROSCOPY

WP 193  UV-Vis Action Spectroscopy and Energetics of Charge-Tagged Adenosine Radicals; Yue Liu; Andy Dang; František Tureček; University of Washington, Seattle, WA

WP 194  REMPI and MATI spectroscopy of non-deuterated and deuterated m-chloro- and m-fluoropyridine; Niklas Heil; Jurgen Grotemeyer; Christian-Albrechts-Univ, Kiel, Germany

WP 195  Differentiation of Hydroxyproline Isomers by Gas-Phase Infrared Ion Spectroscopy of Alkali Metal-Ion Complexes; Baku Acharya; Widana K D N Kaushalya; Amanda Patrick; Mississippi State University, Starkville, MS
**Infrared ion spectroscopy: an alternative for structure identification by NMR?**

Rianne Van Outersterp; Jonathan Martens; Giel Berden; Valerie Koppen; Jos Oomens; Filip Cuypckens; FELIX Laboratory, Radboud University, Nijmegen, Netherlands; Janssen R&D, Beere, Belgium

**Understanding the UV Dependence for Photodissociation of Protonated Methylpyridines Within the UV Region**

Benjamin I. Mckinnon; Samuel J.P. Marton; James P. Bezzina; Stephen J. Blanksby; Adam J. Trevitt; University of Wollongong, Wollongong, Australia; Queensland University of Technology, Brisbane, Australia

**Spectroscopic Identification of Gas-Phased Synthesized Nitrogen-Containing Polycyclic Aromatic Ions**

Oisin J. Shiels; Samuel J.P. Marton; Patrick D. Kelly; Jack Turner; Stephen J. Blanksby; Gabriel Da Silva; Adam J. Trevitt; School of Chemistry and Molecular, University of Wollongong, Wollongong, Australia; Queensland University of Technology, Brisbane, Australia; University of Melbourne, Parkville, Australia

**From isolated self-assembled peptides towards nanostructures: a mass-selective IR action spectroscopy study**

Iuliia Stroganova; Sjors Bakels; Anouk M. Rijs; FELIX Laboratory, Radboud University, Nijmegen, Netherlands

**Rapid IR Spectroscopy and Ion-Packet Enrichment for glycan identification (9/20)**

Ali H Abikhodr; Vasyl Yatsyna; EPFL/LCPM, Lausanne, Switzerland; University of Gothenburg, Gothenburg, Sweden

**Alkali Cation Size-Specific Guest Trapping in Supramolecular Complexes Characterized Using CRAFTI Collision Cross Sections**

Tina H. M. Farzan; Mariah Pay; Brigham Pope; David V. Dearden; Brigham Young University, Provo, UT

**Deprotonated Glycan Dissociation Chemistry**

Jordan M Rabus; Benjamin J Bythell; Ohio University, Athens, OH

**On the Observation of Isomers of Enterobactin and their Fate upon Binding Felli: an Empirical and Theoretical Study**

Daryl Giblin; Lindsey K. Steinberg; Jan M. Crowley; Michael L. Gross; Jeffrey P. Henderson; Washington University, St Louis, MO; Washington University in St.Louis, St.Louis, MO

**Collision Cross-section Measurements of Precursor and Selected Fragmentation Products in Single Experiments by SORI – CRAFTI**

Andrew J. Arslanian; Caleb Tinsley; Noah Mismash; David V. Dearden; Brigham Young University, Provo, UT

**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

**Characterization of Potential Thioredoxin-Mimetic Peptides**

Michael D. Browne; Jianhua Ren; University of the Pacific, Stockton, CA

**Fragmentation pathways of transition metal substituted polyoxovanadates**

Solita Marie Wilson; Ellen M. Matson; Julia Laskin; Purdue University, West Lafayette, IN; University of Rochester, Rochester, NY

**Rapid, quantitative investigation of gas-phase unfolding/dissociation activation enthalpies and entropies for native protein ions**

Micah T Donor; Samantha O. Shepherd; James S Prell; University of Oregon, Eugene, OR


Jamir Shrestha; Caleb Tinsley; Andrew J. Arslanian; Zixuan Feng; Tina H. M. Farzan; Mariah Pay; David V. Dearden; Brigham Young University, Provo, UT; Colorado State University, Fort Collins, CO

**Conformational and Thermochemical Changes of Cysteine Containing Peptides upon Chiral Inversion of Cysteine**

Yuntao Zhang; Jianhua Ren; University of the Pacific, Stockton, CA

**N-Acetyl Glycan Structure and Dissociation Chemistry**

Benjamin Bythell; Shanshan Guan; Jordan M Rabus; Matthew Murphy; John Tschanmpel; Ohio University, Athens, OH; University of Missouri, St. Louis, St. Louis, MO

**An Experimental and Computational Study of the Decomposition of [UO2(O2C-C≡C-CH3)(NO3)2]**

Luke Metzler; Michael Van Stipdonk; Duquesne University, Pittsburgh, PA
**Chemical modification of the matrix gas: Comparison experiments with ESI-MS and ESI-IMS-MS:**
Christine Polaczek; Christian Thoben; Maria Allers; Stefan Zimmermann; Thorsten Benter; University of Wuppertal, Wuppertal, Germany; Leibniz University Hannover, Institute of Electrical Engineering and Measurement Technology, Hannover, Germany

**Factors that affect the formation of multiply charged protein ions in a MALDI process:**
Avinash Adhikrao Patil; Thi Khanh Ly Lai; Cheng-Kang Chiang; Wen-Ping Peng; National Dong Hwa University, Shoufeng, Taiwan

**Discrimination of position isomers of benzene derivatives based on TOF mass spectra derived using femtosecond laser ionization:**
Kennesuke Hoshina; Tatsuro Shirota; Niigata University of Pharmacy and Applied Life Sciences, Niigata, Japan

**Towards Higher Throughput in LC-MS - DB-nESI Overcomes the Ion Flux Problem of Modern Instruments:**
Sebastian Brandt; Michael Schilling; Albert Sickmann; Joachim Franzke; Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany; University of Aberdeen, Department of Chemistry, Aberdeen, United Kingdom; Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany

**Microwave-Assisted Electrospray Ionization:**
Steven Ray; Maria Rivera; University at Buffalo, SUNY, Buffalo, NY

**Influence of Matrix Crystal Size on the Plume Effective Temperature in MALDI:**
Lee Elliott; Gary R. Kinsel; Mary E. Kinsel; Southern Illinois University Carbondale, Carbondale, IL

**New Insights Relative to Matrices in Mass Spectrometry:**
Milan Pophristic; Khoa Hoang; Charles N Mcewen; MSTM LLC, Newark, DE

**Unexpected EI fragmentations: Loss of tetramethylsilane in vicinal TMS diols; Transfer of an acetyl group across an aromatic amino alcohol:**
N. Rabe Andriamaharavo; H. Martin Garraffo; Stephen E. Stein; National Institute of Standards and Technology, Gaithersburg, MD

**Rearrangement of TMS of halogenated 1-phenylethanone and related compounds in EI Mass Spectra:**
Yufang Zheng; H. Martin Garraffo; Weihua Ji; Stephen E. Stein; NIST, Gaithersburg, MD

**Rearrangement of the TMS ester of 4-Oxo-4H-chromene-2-carboxylic acid and analogs in EI mass spectra:**
Yufang Zheng; H. Martin Garraffo; N. Rabe Andriamaharavo; Stephen E. Stein; National Institute of Standards and Technology, Gaithersburg, Maryland

**Characterization of glycerides and other impurities in biodiesel by high temperature gas chromatography combined with isobutane chemical ionization mass spectrometry:**
Roza Wojcik; Tessa L Oxford; Cherylyn W Wright; Angela M Melville; Bob W Wright; PNNL, Richland, WA

**Thermal Desorption Coupled Gas Chromatography-Mass Spectrometry Analysis of Low Emission Polyurethane Foam for Automobile Applications:**
Yuling Tan; Adam Grzesiak; Eric Pearce; Gavin Marr; Michael Donate; Kelly Kiszka; The Dow Chemical Company, Midland, MI

**Comparison of extracted and non-extracted calibration curves in the GC-MS determination of method detection limits for haloacetonitriles:**
George William Kajjumba; Tammy Jones-Lepp; Meena Ejada; Erica J Marti; University of Nevada, Las Vegas, Las Vegas, NV; Department of Civil and Environmental Engineering and Construction, Las Vegas, NV

**Development and validation of an improved, TF-SPME based, standard gas generating vial for the repeatable generation of headspace standards:**
Jonathan J Grandy; Khaled Murtada; João R Belinato; Janusz Pawliszyn; University of Waterloo, Waterloo, ON; Institute of Chemistry, University of Campinas, Campinas, Brazil; National Institute of Science and Technology in Bioanalysis (INCTBio), Campinas, Brazil

**Inferring the molecular mass of an analyte from its electron ionization mass spectrum:**
Arun S Moorthy; Anthony J Kearsley; W Gary Mallard; William E Wallace; Stephen E Stein; NIST, Gaithersburg, MD

**Identification and quantification of the phytosterols in Korean maize (Zea mays L.) F1 hybrids using Gas Chromatography-mass spectrometry:**
Dong Yeol Lee; Won Min Jeong; Hyeong Hwan Lee; Jong Soo Ryu; Tae Wook Jung; Sang Gon Kim; Gyeongnam Oriental Anti-Aging Institute, Sancheong-gun, South Korea; National Institute of Crop Science, Miryang, South Korea
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 Majula1; Anthony Debastiani1; Sara Macios1; Kushani Attanayake2; Stephen J Valentine1; 1West 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); Rajashkekar Kammari1; Jainik P. Panchal2; Brent Kochert3; Sneet Deshmukh2; Elizabeth M. Topp1; 1Department of Industrial and Physical Pharmacy, College of Pharmacy, Purdue University, West Lafayette, IN; 2Sterile Formulation Sciences, Merck & Co., Inc., Kenilworth, NJ; 3AR&D Mass Spectrometry, Merck & Co. Inc., Kenilworth, NJ

WP 232  Organic Solvents on the HDX Platform for Efficient Denaturation; Chunyang Guo1; Ming Cheng2; Lindsey K. Steinberg3; Jeffrey P. Henderson4; Michael L. Gross5; WUSTL, St. Louis, MO; 2The Scripps Research Institute, La Jolla, CA; 3Washington University in St.Louis, St.Louis, MO; 4Washington University, St Louis, MO

WP 233  The Deuterium Calculator: An open-source software for hydrogen-deuterium exchange mass spectrometry analysis; Thomas Welborn1; Kellye Cupp-Sutton1; Zhe Wang1; Si Wu1; Kenneth Smith2; 1University of Oklahoma, Norman, OK; 2Oklahoma 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. Grande1; David D. Weis2; 1University of Kansas, Lawrence, KS

WP 235  Hydrogen/deuterium exchange mass spectrometry (HDX-MS) for complex sample analysis; Mulin Fang1; Zhe Wang1; Thomas Welborn1; Kellye A. Cupp-Sutton1; Kenneth Smith2; Si Wu1; 1University of Oklahoma, Norman, OK; 2Oklahoma Medical Research Foundation, Oklahoma City, OK

WP 236  Supercharging for Improved ECD/ETD-Based Hydrogen/Deuterium Exchange Mass Spectrometry of Biotherapeutics; Leeanne Wang1; Qingyi Wang1; Kristina Håkansson1; 1Department 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 Kim1; Darren T. Gass2; Elyssia S. Gallagher1; 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 Largy1; Valérie Gabelica1; 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. Petrochenko1; Konstanin I. Popov2; Christoph H. Borchers1,3,4; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia

WP 241  Imidazolyl Compounds as Internal Exchange Reporters for Hydrogen/Deuterium Exchange by Mass Spectrometry; Taylor A Murprhee1; Clint Vorauer1; Marie Brzoska1; Miklos Guttmann1; 1University of Washington, Seattle, WA

WP 242  Fundamentals of Gas-Phase Hydrogen Deuterium Exchange (gHDX) and Implications for Structural Elucidation of Small Molecules; Sanjit S. Upal (Sunny)1,2; Abhiyoga Mookherjee1,2; Rick Harkewicz1,2; Sarah E. Beasley1,2; Matthew F. Bush1,3; Miklos Guttmann1,2; 1University of Washington, Seattle, WA; 2Department of Chemical Medicine, University of Washington, Seattle, WA; 3Department of Chemistry, University of Washington, Seattle, WA

WP 243  Performance Evaluation of Hydrogen Deuterium Exchange on a Waters Synapt XS; Lindsay Morrison1; Barbara J Sullivan1; 1Waters 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. Wollenberg1,2; Stuart Pengelly3; Jeppe C. Mouritsen1; Detlev Suckau4; Christian I. Jorgensen1; Thomas J. D. Jorgensen2; 1Novozymes A/S, Kgs. Lyngby, Denmark; 2University of Southern Denmark, Odense M, Denmark; 3Bruker Daltonic GmbH, Bremen, Germany

WP 245  In-electrospray H/D Exchange of Carbohydrates Using a D2O/N2Gas Infusion System; Ana V. Quintero1; O. Tara Liyanage1; Chinthaka A. Seneviratne2; Elyssia S. Gallagher1; 1 Baylor University, Waco, TX; 2Mass Spectrometry Center, Baylor University, Waco, TX

WP 246  HDXmodeller: an online webservice for high-resolution HDX-MS with auto-validation; Antoni James Borysik1; Ramin Eghteiari Salmas1; 1King's College London, London, United Kingdom
Development of a Novel Ion Imaging Unit toward Microscope Mode Mass Spectrometry Imaging: Tsuyoshi Hirao1, 2; Hajime Nishimura2; Yasuhide Naito1; 1The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan; 2Hamamatsu Photonics K.K., Iwata, Japan

Comparative N-glycome analysis of prostate cancer tissues using MALDI-Q-TOF versus MALDI-FTICR imaging mass spectrometry workflows: Grace Grimley1; Connor A West1; Xiaowei Lu1; Anand S Mehta1; Peggi M Angel1; Richard R Drake1; 1Medical University of South Carolina, Charleston, SC

Sub-micron 3D SIMS imaging combined with automated, high mass resolution MS/MS: Alexander Pirkl1; Henrik Arlinghaus2; Daniel Breitenstein3; Karsten Lamann4; Elke Tallarek2; Birgit Hagenhoff4; Ewald Niehuis1; 1IONTOF Technologies GmbH, Muenster, Germany; 2IONTOF Technologies GmbH, Muenster, Germany; 3TASCON GmbH, Muenster, Germany; 4TASCON GmbH, Muenster, Germany

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 Cocbic1; Jens Soltwisch2 3; Bram Heij3 4; Annika Koch5; Karl Smith6; Klaus Dreisewerd7; C. Logan Mackay7; Kingdom; 2University of Manchester, Manchester, United Kingdom; 3University of Manchester School of Pharmacy, Manchester, United Kingdom; 4Queensland University of Technology, Brisbane, Australia; 5SIRCAMS, Edinburgh, United Kingdom

From Tissue Imaging to Cancer Surgery – Utilisation of Laser Desorption – Rapid Evaporative Ionisation Mass Spectrometry: Daniel Simon1; Julia Abda1; Hanifa J.A. Koguna1 2; Stefania M. Stavrakaki1;olf Isberg1; Julia Balog2; Tamas Karancsi3; Josephine Bunch1 2; Zoltan Takats1; 1Waters Corporation, Wilmslow, United Kingdom; 2Queensland University of Technology, Brisbane, Australia

A Dual SIMS / MALDI Source for an Orthogonal TOF Imaging Mass Spectrometer: Ian G. M. Anthony1; Joel D. Keelor2; Sebastian Böhm3; Shane R. Ellis4; Claus Köster5; Jens Hoehndorf6; Ron M.A Heeren1; 1IONTOF Technologies GmbH, Muenster, Germany; 2Hamamatsu Photonics K.K., Iwata, Japan; 3TASCON GmbH, Muenster, Germany; 4TASCON GmbH, Muenster, Germany; 5Bruker Daltonik GmbH, Bremen, Germany

Using Ozone-Induced dissociation to demonstrate varying distribution patterns of unsaturated Isobaric lipids by DESI imaging Mass Spectrometry: Mark Towers1; Lisa Reid1; Berwyck Poad2; Martin Green1; Emmanuelle Claude1; 1Waters Corporation, Wilmslow, United Kingdom; 2Queensland University of Technology, Brisbane, Australia

High-throughput ion microscope imaging using the time-stamping Timepix3 sensor: Natasha M Smith1; Robert Burleigh1; Daniel Wood1; Ang Guo1; Michael Burt1; Ian Shipsey1; Daniela Bortoletto1; Richard Plackett1; Mark Brouard1; 1University of Oxford, Oxford, United Kingdom

Design and characterization of novel sprayer for high resolution tissue imaging by desorption electrospray ionization (DESI): Stephen J Hattan1; Presha Rajbandari2; Brandon Fowler2; Fereshte Zandkarimi2; Brent R. Stockwell2; Gregory Roman1; Wade Leveille1; Jeffrey Musacchio1; Ashwin Meyyappan1; Jim Murphy1; Joseph Michienzi1; Emrys Jones1; Steven Pringle1; 1Waters Corporation, Milford, Massachusetts; 2University of Wollongong, Wollongong, Australia; 3Bruker Daltonik GmbH, Bremen, Germany; 4TASCON GmbH, Muenster, Germany

Development of a Multimodal Fully Integrated Imaging Platform using Infrared Laser-Assisted REIMS and DESI for High Throughput Slide analysis: Istvan Pap1; Richard Schaffer1; Csaba Hajdu1; Daniel Simon4; Tamas Karancsi1; Julia Balog3; 1Waters Research Center, Budapest, Hungary; 2Imperial College London, London, United Kingdom

Desorption Electrospray Ionisation Imaging on the Cyclic Ion Mobility-Mass Spectrometry System: Emrys A Jones1 2; Matthew Gentry2; Jakub Ujma1; Robert Tonge1; Danielle Mcdougall2; James I Langridge1; Adam Mcmahon1; 1Waters Corporation, Wilmslow, United Kingdom; 2University of Manchester, Manchester, United Kingdom

MALD-MSI Evaluation of Penetration of Different Pyrazole-based Compounds into Multicellular Tumor Spheroids: Yijia Wang1; Yong A2; Fengtian Xue2; Amanda B. Hummon1; 1The Ohio State University, Columbus, OH; 2University of Maryland School of Pharmacy, Baltimore, MD

Non-targeted exploration of metabolic processes and xenobiotic metabolism in plants exposed to micropollutants using mass spectrometry imaging: Claire Villette1; Alexandre Verdue2; Aiko Barsch2; Nikolas ASMS 2020 Reboot
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The absorption of drugs through porcine gastrointestinal tissue analysed by mass spectrometry imaging; Chloe E Spencer1; Stephen Rumbley2; Steven Mellor2; Catherine Duckett1; Malcolm R Clench1; 1BMRC, Sheffield Hallam University, Sheffield, United Kingdom; 2CRODA Inc (B88), New Castle, DE19720; 3CRODA Europe Ltd, Leek, United Kingdom

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4D-Lipidomics based automated annotation of MALDI Imaging data using a dedicated bioinformatics pipeline; Janina Oetjen1; Christian Marschling2; Sven W. Meyer1; Corinna Henkel1; Annika Koch1; Nikolaus Kessler1; Wiebke Timm1; Aiko Barsch1; Jan H. Kobarg1; Dennis Trede1; Heiko Neuweger1; Carsten Hopf1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim Technical University, Mannheim, Germany

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Effect of CO-inhibition on the lipid change in early pregnancy in mice; Éva Szabó1; Stefania Gitta1; Janos Schmidt1; Laszlo Mark1; 1Institute 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; Caitlin Tressler1; Hong Liang1; Katherine Stumpo2; James R. Eshleman1; Kristine Glunde1; 1Johns Hopkins University School of Medicine, Baltimore, Maryland; 2University of Florida Department of Chemistry, Gainesville, FL, 3University of Scranton, Scranton, PA

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Mass Spectrometry Imaging to Evaluate the Role of Sulfatide in NeuroHIV; Daniela D’amo1co1; Eliseo Eugenie1; Brentand Prideaux1; 1UTMB, Galveston, TX

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Understanding Mitragyna speciosa alkaloid metabolism and pharmacology in rat brain using imaging mass spectrometry; Zhongling Liang1; Orelia Ceriati1; Tamara I. King1; Abhisheak Sharma2; Christopher R. McCurdy2; Boone M. Prentice1; 1University of Florida Department of Chemistry, Gainesville, FL; 2University of Florida, Gainesville, FL

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Lipid Distribution in Liver Is Disrupted in the Translocator Protein (TSPO, 18-KDa) Knockout Mouse Model; Cristina I Silvescu1; Li Yuchang2; Chantal Sottas2; Junji Watanabe2; Jeremy Wolff1; Shannon Cornett1; Vassilios Mccurdy2; Boone M. Prentice1; 1Bruker Scientific LLC, Billerica, MA; 2School of Pharmacy, University of Southern California, Los Angeles, CA

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Metabolite Explorer: a software tool for targeted analysis of mass spectrometry imaging data; Thomas Moerman1; Michael Becker1; Nico Verbeek1; 1Institute for Hygiene, University of Muenster, Muenster, Germany; 2Institute 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; 3Institut des Sciences Analytiques, Universite Claude Bernand, Villeurbanne, France; 4Cubé Laboratoire des sciences de l’ingenieur, de l’informatique et de l’imagerie, Strasbourg, France

WP 269
A study of drug metabolism using a zebrafish larvae model and MALDI-MS Imaging; Yu Mi Park12; Jennifer Herrmann3, 4; Daniel Krug1, 4; Aiko Barsch1; Nikolaus Kessler1; Alice Ly6; Jan H. Kobarg1; Tingting Fu1; Tingting Fu2; Janina Oetjen1; Christian Marschling2; Sven W. Meyer1; Corinna Henkel1; Annika Koch1; Nikolaus Kessler1; Wiebke Timm1; Aiko Barsch1; Jan H. Kobarg1; Dennis Trede1; Heiko Neuweger1; Carsten Hopf1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim Technical University, Mannheim, Germany

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In situ isobaric and isomeric lipid mapping and identification by MALDI-Ion Mobility Separation-Mass Spectrometry Imaging; Tingting Fu1; Janina Oetjen1; Samuel Chapelle2; Alexandre Verdue2; Matthias Szesny2; Arnaud Chaumot2; Davide Degli-Esposti2; Olivier Geffard2; Yohann Clément1; Arnaud Salvador1; Nannan Tao4; Sophie Ayciriex1; 1Institut des Sciences Analytiques, Universite Claude Bernand, Villeurbanne, France; 2Bruker Daltonik GmbH, Bremen, Germany; 3Tritea, UR RiverLy, Laboratoire d’écotoxicologie, Villeurbanne, France; 4BMRC, Sheffield Hallam University, Sheffield, United Kingdom; 4Bruker Daltonik, Bremen, Germany; 5Bruker Daltonics, San Jose, CA, United States

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High Throughput and High Sensitivity Isomer-resolved Imaging of Lipids by Integration of Ozone-induced dissociation with a MALDI-QTOF Mass Spectrometer; Andrew Bowman1; Britt S. R. Claes1; Berwyck Poad2;
WP 275  Comprehensive analysis of metabolites and biomarkers in lung using MALDI-MSI and DESI-MSI; William Temple Andrews¹; Amanda Oglesby-Sherrouse¹; Angela Wilks¹; Ann M Farese²; Thomas J MacVittie²; Maureen A Kane¹; ¹University of Maryland School of Pharmacy, Baltimore, MD; ²University of Maryland School of Medicine, Baltimore, Maryland

WP 276  Integrating high resolution MALDI imaging into the development pipeline of anti-Tuberculosis drugs; Axel Treu¹; Julia Kokesch-Himmelreich¹; Alan Race¹; Kerstin Walter²; Christoph Hölscher²; Andreas Römpp¹; ¹Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; ²Infection 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 Yasui¹; Kohta Yamamoto²; Daiki Kameyama³; Takashi Nirasawa⁴; Ryo Kajita⁴; Nobuto Kakuda³; Takafumi Hirata²; Masaya Ikegawa³; ¹Doshisha University, Kyotanabe, Japan; ²Geochemical Research Center, The University of Tokyo, Japan; ³Doshisha University, Kyotanabe, Japan; ⁴Bruker Japan K.K., Yokohama, Japan
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 Vrolijk1, 2; Madhushri Shrikant Varunjikar3; Josef Daniel Rasinger3; Benjamin Neely4, 5; Magnus Palmblad6; 1Leiden University Medical Center, Leiden, Netherlands; 2University of Applied Sciences, Leiden, Netherlands; 3Institute of Marine Research, Bergen, Norway; 4National Institute of Standards and Technology, Charleston, SC; 5Hollings Marine Laboratory, Charleston, SC; 6Leiden University Medical Center, Leiden, Netherlands

WP 279  LC-MS ESI Parameter Optimization with Bayesian Optimization for High Sensitivity Measurement; Yusuke Tagawa1; Yuki Ishikawa1; Mikael Levi1; Wataru Fukui1; Jun Watanabe1; Hisanori Morita1; 1Shimadzu corporation, Kyoto, Japan

WP 281  A New Approach to Estimate Protein-Protein Interactions using Proteomics Data; Ahmad Borzou1; Rovshan G. Sadovy1; 1UTMB, Galveston, TX

WP 282  EnvCNN: A Convolutional Neural Network Model for Evaluating Isotopomer Envelopes in Top-Down Mass-spectral Deconvolution; Abdul Rehman Basharat1; Zhe Wang2; Rachele Lubecky3; Si Wu2; Liangliang Sun3; Xiaowen Liu1; 1Indiana University - Purdue University Indianapolis, Indianapolis, IN; 2University of Oklahoma, Norman, OK; 3Michigan State University, East Lansing, MI

WP 283  A new algorithm for fast, parameter-free extraction of ion chromatograms; Rob Smith1, 2; Mathew Guiterrez1, 2; 1University of Montana, Missoula, MT; 2Prime Labs, Inc., Missoula, MT

WP 284  LC-MS correspondence using a feature-aware, direct match approach without retention time alignment; Michael Callahan1, 2; Rob Smith1, 2; 1Prime Labs, Inc., Missoula, MT; 2University of Montana, Missoula, MT

WP 285  Identification of Cutibacterium acnesby machine learning using amino acid sequence information; Tatsuki Okubo1; Kanae Teramoto1; Yoshihiro Yamada1; Sadanori Sekiya1; Shinichi Iwamoto1; Koichi Tanaka1; 1Shimadzu corporation, Kyoto, Japan

WP 286  Fast deisotoping algorithm and its implementation in MSFragger search engine; Guo Ci Teo1; Daniel Polasky1; Fengchao Yu1; Alexey I. Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

WP 287  JUMPo: ordinal-differential equation-based protein turnover modeling of mass spectrometric data from metabolically labeled animals; Surendhar Reddy Chepalya1; Xueyan Liu2; Alex M. Breuer1; Zhiping Wu1; Ji-Hoon Cho1; Aniana Mancieni1; Yun Jiao1; Hui Zhang1; Junmin Peng1; 1St. Jude Children’s Research Hospital, Memphis, TN; 2University of New Orleans, New Orleans, LA; 3Northwestern University, Chicago, IL

WP 288  PRiSM: exhaustive and agnostic database searching; Joris Van Houtven1; Kurt Boonen2; Geert Baggerman2; Kris Laukens3; Jef Hooyberghs4; Dirk Valkenborg1; 1Hasselt University, Hasselt, Belgium; 2Centre for Proteomics, Antwerp; Belgium; 3Biomina, Antwerpen, Belgium; 4VITO, Mol, Belgium

WP 289  Peptide profiling and predictive modelling of dairy products throughout fermentation; Fionnuala Murphy1, 2, 3; Stefan Clerens1, 3, 4; Esther Meenken1; Julie Dalziel1, 2; Joanne Hort2, 3; Julia Low2, 3; 1AgResearch, Christchurch, New Zealand; 2Massey University, Palmerston North, New Zealand; 3Riddet Institute (Massey University), Palmerston North, New Zealand; 4Biomolecular Interaction Centre (Canterbury University), Christchurch, New Zealand

WP 290  Clustering of spectra renders improved, automated identification and quantification of glycan structures; Christopher Ashwood1; Matthew The2; Rebekah L Gundry3; Lukas Kall3; 1CardiOms 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; 2Technical University of Munich (TUM), Freising, Germany; 3Royal Institute of Technology, Stockholm, Sweden

WP 291  Floodlight and Searchlight: Innovative Software for Machine Learning Assisted Data Reduction and Pattern Analysis; Kristin A Favela1; Michael J Hartnett2; Andrew J Schaub1; Jake A. Janssen1; Adam K Van Horn1; David W Vickers1; Keith S Pickens1; 1Southwest Research Institute, San Antonio, TX

WP 292  Mobilatron: software framework for signal extraction from ion mobility enabled mass spectrometry data; Dmitry Avtonomov1; Sarah E. Haynes1; Daniel A. Polasky1; Carolina Rojas Ramirez1; Brandon T. Ruotolo1; Alexey I. Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

WP 293  CoreMS: Open Source Mass Spectrometry Software Framework for Small Molecules Analysis; Yuri E. Corilo1; Allison M. Thompson1; William Kew1; Lisa M Bramer1; Lee Ann McCue1; 1Pacific Northwest National Laboratory, Richland, WA

WP 294  Correctly controlling false discovery rates in targeted database searches; Andy Lin1; Uri Keich2; William Stafford Noble1; 1University of Washington, Seattle, WA; 2University of Sydney, Camperdown, Australia
WEDNESDAY POSTERS (WP) Pges 86-124 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

WP 295 Improvements in Two-Dimensional GCxGC Data Alignment by a Supervised Learning Guided Approach for Automated Peak Comparisons; Andrew J Schaub; Jake A. Janssen; Michael J Hartnett; Kristin A Favela; Adam K Van Horn; David W Vickers; Keith S Pickens; Southwest Research Institute (SwRI), San Antonio, TX

WP 296 Accelerated Isotopic Envelope Calculations using IsoSpec; Michal P. Startek; Dirk Valkenberg; Mateusz Krzysztof Lacki; University of Warsaw, Warsaw, Poland; Hasselt University, Hasselt, Belgium; University Medical Center, Johannes Gutenberg University, Mainz, Germany

WP 297 MSstatsSampleSize: Simulation tool for optimal design of high-dimensional MS-based proteomics experiments; Ting Huang; Meena Choi; Tiannan Guo; Sumedh Ravikant Sanke; Yansheng Liu; Matthew Tham; Ruedi Aebi; Northeastern University, Boston, MA; Westlake University, Hangzhou, China; Yale University School of Medicine, West Haven, CT; ETH Zurich, Zurich, Switzerland; University of Zurich, Zurich, Switzerland

WP 298 Repository-scale queries of MS/MS spectra; Benjamin Pullman; Nuno Bandeira; UC San Diego, La Jolla, CA; 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; Yu-Meng Ou; Shu-Yun Kuo; Yi-Sheng Wang; Genomics Research Center, Academia Sinica, Taipei, Taiwan

WP 300 Science Autonomy and the ExoMars Mission: Machine Learning to Help Find Life on Mars; Victoria Da Poian; Eric Lyness; William B Brinkerhoff; Ryan M. Danel; Desmond Kaplan; Xiang Li; Melissa G. Trainer; NASA Goddard Space Flight Center, Greenbelt, MD; Danell Consulting, Inc., Winterville, NC; KapScience LLC, TEWKSBURY, MA; University of Maryland Baltimore County, Baltimore, Maryland

WP 301 Masserstein: A Python package for a robust linear deconvolution using optimal transport; Michal Ciach; Grzegorz Skoraczynski; Szymon Majewski; Michal P. Startek; Blażej Miascojedow; Dirk Valkenberg; Anna Gambin; University of Warsaw, Warsaw, Poland; Institute of Mathematics, Polish Academy of Sciences, Warsaw, Poland; Hasselt University, Hasselt, Belgium

WP 302 The MasSpOT - Optimal Transport for Mass Spectrometry; Grzegorz Skoraczynski; Blażej Miascojedow; Szymon Majewski; Anna Gambin; Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; Institute of Mathematics, Polish Academy of Sciences, Warsaw, Poland

WP 303 Utilizing conditional probability distributions to identify peptides that contain heavy isotopes; Jonathon O'Brien; Phillip Setzler; Nicole Haste; Celeste M. Sandoval; Yao Wong; Ramin Rad; Aleksandr Gaun; Carmela Sidrauski; Vladimir Jojc; Fiona E. Mcallister; Bryson D. Bennett; Calico Life Sciences LLC, South San Francisco, California

INFORMATICS: MULTIOMICS INTEGRATION

WP 304 ProteomicsDB: Integrating drug targets, phenotypes and expression data; Patroklos Samaras; Tobias Schmidt; Marwin Shraideh; Ludwig Lautenbacher; Martin Frejno; Siegfried Gessulat; Jana Zecha; Anna Jarzab; Maria Reinecke; Stephanie Heinzleim; Johannes Rank; Helmut Kremer; Bernhard Kuster; Mathias Wilhelm; Technical University of Munich (TUM), Freising, Germany; Technical University of Munich (TUM), Garching, Germany

WP 305 Comprehensive Proteogenomic Analysis of Peptides and Proteoforms with MetaMorpheus; Rachel M Miller; Anthony J. Cesnik; Robert J Millikin; Michael R. Shortreed; Lloyd M Smith; University of Wisconsin-Madison, Madison, Wisconsin; Stanford University, Stanford, CA; 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; Jonathan T Lei; Eric J Jaehnig; Bing Zhang; Baylor College of Medicine, Houston, TX

WP 307 Proteomic data commons: a resource for proteogenomic analysis; Ratna Rajesh Thangudu; Michael Holck; Deepak Singh; Paul A Rudnick; Michael J MacCors; Nathan J Edwards; Karen A Ketchum; Christopher R Kinsinger; Erika Kim; Anand Basu; ESAC, Inc., Rockville, MD; Spectragen Informatics, Bainbridge Island, WA; University of Washington, Seattle, WA; Georgetown Univ., Washington, DC; National Cancer Institute, Bethesda, MD

WP 308 Integrative transcriptome, proteome, and phosphoproteome reveal new aspects of high productivity in CHO cells; Prashant Kaushik; Vijay Tejwani; Shangzhong Li; Michael Henry; Nathan E. Lewis; Paula Meade; Susan T. Shafirstein; National Institute for Cellular Biotechnology, Dublin City University, Dublin, Ireland; Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, NY; Department of Bioengineering, University of California, San Diego, La Jolla, CA; Novo Nordisk Foundation Center for Biosustainability, University of California, San Diego, La Jolla, CA; 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 Ahn1; Junhyuk Song2; Sunyoung Seo2; Jiyoung Yu3; Jeonghun Yeom1; Hyunghee Kim1; Sangyong Jon1; Kyunggon Kim1,2; 1Asan Medical Center, Seoul, South Korea; 2Korea Advanced Institute of Science and Technology, Daejeon, South Korea; 3Korea University, Seoul, South Korea; 4Korea University, Seoul, South Korea; 5Korea Advanced Institute of Science and Technology, Daejeon, South Korea; 6University of Ulsan, Seoul, South Korea

WP 310 Alomic: An Artificial Intelligence (AI) enabled integrative Omics pipeline; Raghav Sehgal1; Giushi Sun1; Rebecca Cardone1; Richard Martyn Williams1; Xiaojian Zhao1; Surbhi Poddar2; Richa Mudgal2; Richard Schneider3; Richard G. Kibbey1; 1Yale University, New Haven, CT; 2Elucidata, Delhi, India; 3NCATS/NIH, Rockville, MD

WP 311 Robust In Silico Fractionation of Diverse Molecular Ion Adduct Forms in Positive- and Negative-Ion Mode ESI; Luke T. Richardson1; Shubhnuteet Warar1; Touradj Solouki1; 1Baylor University, Waco, TX

WP 312 Evaluating customized database generation methods for metaproteomics analysis; Subina Mehta1; Thomas Mccowan1; James E Johnsson1; Praveen Kumar1; Magnus O Arnzen2; Francesco Delogu2; Marie A Crane3; Peter S Thuy-Boun1; Dennis W Woolan4; Timothy J Griffin1; Pratik Dilip Jagtap1; 1University of Minnesota, Minneapolis, MN/55455; 2Norwegian University of Environmental and Life Sciences, Ås, Norway; 3Macalester College: Private Liberal Arts College, St. Paul, Minnesota; 4The Scripps Research Institute, La Jolla, CA

WP 313 ImmuNOVO: An integrated platform for neoantigen discovery based on immunopeptidomics and genomic data; Sujin Li1; Yue Qi2; Udayan Guha3; Haixu Tang1; 1Indiana University, Bloomington, IN; 2Thoracic & Gastrointestinal Oncology Branch, Center for Cancer Research, NCI, Bethesda, MD

WP 314 Integrated genome and metabolome analysis highlighting the role of Glucagon-like Peptide 1 signaling and other pathways in increasingly severe asthma; Jalal Siddiqui1; Tara Eicher2; Rachel Kelly2; Raghu Machiraju1; Juan Celedon1; Scott Weiss2; Jessica Lasky-Su2; Ewy Mathe1; 1The Ohio State University, Columbus, OH; 2Brigham and Women’s Hospital, Harvard Medical School, Boston, MA; 3University of Pittsburgh, Pittsburgh, PA

WP 315 SysMet: A Suite of Tools for Integrative Systems Metabolomics; Mohammad R Nezami-Ranjarb1; Linge Yan1; Habtom W Ressoon3; 1OmisCraft, Washington, District of Columbia

WP 316 Numerical and a priori knowledge-driven methods for integrating metabolomics data with other omics data; Andrew Patt1; Tara Eicher2; Elizabeth Baskin1; Bofei Zhang3; Joseph Mcelroy1; Kevin Coombes1; Ewy Mathe1; 1Ohio State University Medical Center, Columbus, OH; 2Ohio State University, Columbus, Ohio; 3New 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 Kwan1; Ben Tin-Yong Wong2; Anna Xiao-Dan Yu1; Tina Ting-Xia Dong1; Henry Hei-Ning Lam2; Karl Wah-Keung Tsim1; 1Division of Life Science and Center for Chinese Medicine, The Hong Kong University of Science and Technology, Kowloon, China; 2Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Kowloon, China

WP 319 Omni-MS: application of a one-shot multomic data for prediction of multiple clinical biomarkers and diagnoses; Austin Quach1; Alexander Yoon1; Whitaker Cohn1; Julian P Whitelegge1; 1UCLA 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 Abramchuk1; Karen E. Wei2; Lizbeth-Carolina Aguilar2; Alexander Ratushny3; Michael P. Rout1; John D. Aitchison3; Kevin Coombes1; Ewy Mathe1; 1Baylor University, Waco, TX; 2Ohio State University Medical Center, Columbus, OH; 3University of Pittsburgh, Pittsburgh, PA

WP 321 OmicLoupe: Interactive visualizations of differential expression comparisons across omics datasets; Jakob Willforss1; Fredrik Levander1; 1Lund University, Department of Immunotechnology, Lund, Sweden

WP 322 Data Independent Acquisition using Dual Linear Ion Trap (LIT) Miniature Mass Spectrometer; Nan Wang1; Zhijun Cai2; Zheng Ouyang1; 1Department of Precision Instrument, Tsinghua University, Beijing, China

WP 323 Transportable Mass Spectrometer for Rapid Analysis of Nuclear Material and Environmental Samples; Ankur Chaudhuri1; Liqian Li1; James Johnston1; Martin-Lee Cusick1; 1Canadian Nuclear Laboratories, Chalk River, ON

WP 324 MAss Spectrometer for Planetary EXploration – ORGANic Composition Analyzer (MASPEX-ORCA) for Europa Lander; Ryan C. Blase1; Chris Glein1; Mark Libardoni1; Kelly Miller1; Hunter Waite1; Gregory Miller1; Kate Craft2; Chris Bradburne2; Korine Ohiri2; Mark Perry2; Tessa Vanvolkenberg2; Katsuo Kurabayashi3; Xudong Fan3; Hongbo Zhu3; Anandram Venkatasubramanian3; Abhishek Ghosh3; Peter Wurz3; Rico Fausch4; 1Southwest
**WP 325**

Direct on-site screening of fentanyl analogues using matrix-assisted ionization vacuum on a miniature mass spectrometer; Xiangyu Guo1; Yuhan Shang1; Hua Bai1; Qiang Ma1; 1Chinese 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. Gamage1; Daniel E. Austin1; 2Brigham Young University, Provo, UT

**WP 327**

Study on the Thermal Expansion Effects of the ceramic high-resolution multiple electrodes harmonized Kingdon trap; Anastasiia Fursova1; Oleg Kharybin1; Gleb Vladimirov1; Eugene (evgeny) Nikolaev2; 1Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; 2Skolkovo institute of science and technology, Moscow Region, Russian Federation

**WP 328**

“Brick” Mass Spectrometer: catch up lab-scale MS and beyond; Qian Xu1; Ting Jiang1; Zuqiang Xu2; Yang Tang1; Yanbing Zhai1; Wei Xu1; 1Beijing Institute of Technology, Beijing, China; 2Beijing Institute of Technology, Beijing, China

**WP 329**

Characterization of Capillary Electrophoresis-Electrospray Ionization Performance of the Europen Molecular Indicators of Life Investigation (EMILI) Mass Spectrometer; Desmond A Kaplan1, 2; Ryan M Danell1, 3; Xiang Li1, 4; Marco E Castillo1; Ryan Danell1; Desmond Kaplan1; Stephanie A Getty1; Andrej Grubisic1; William B Brinckerhoff1; Paul R Mahaffy1; Eric Lyness1; And The Moma Team1; 1Mini-Mass Consulting, Inc, Hyattsville, MD; 2University of Maryland Baltimore, Baltimore, MD; 3NASA Goddard Space Flight Center, Greenbelt, MD; 4ATA Aerospace, Greenbelt, MD 20770; 5Danell Consulting, Inc., Winterville, NC; 6University of Maryland Baltimore, Baltimore, MD; 7Mini-Mass Consulting Inc., Hyattsville, MD; 8NASA Jet Propulsion Laboratory, Pasadena, CA

**WP 330**

MOMA Mass Spectrometer Laser Desorption Ionization of Mineral Samples; Friso H.w. Van Amerom1; Xiang Li2, 3; Marco E Castillo4; Ryan Danell1; Desmond Kaplan1; Friso H.w. Van Amerom1; 1Brigham Young University, Provo, UT; 2University of Maryland Baltimore, Baltimore, MD; 3NASA Goddard Space Flight Center, Greenbelt, MD; 4ATA Aerospace, Greenbelt, MD 20770; 5Danell Consulting, Inc., Winterville, NC; 6KapScience LLC, TEWKSBURY, MA; 7Danell Consulting, Inc., Winterville, NC; 8KapScience LLC, TEWKSBURY, MA; 9Microtel LLC, Greenbelt, MD; 10Max Planck Institut für Sonnensystemforschung, Goettingen, Germany

**WP 331**

Development of MEMS-based Gas Sample Collector for a Fieldable Miniature GC-MS Instrument; Vladimir M. Doroshenko1; Victor Laiko1; Eugene Moskovets1; Constantin Novoselov1; Tzu-Hsuan Chang2; Daniel Struk1; Jean-Marie D. Dimandja2; Seung Joon Paik2; Milad Navaei2; Peter J. Hesketh3; 1MassTech, Inc., Columbia, MD; 2Georgia Institute of Technology, Atlanta, GA

**WP 332**

Micro Ion Trap Array for Portable GC/MS Analysis of Chemical Vapors; Michael S. Wei1; Ashish Chaudhary1; Strawn Toler1; R. Timothy Shot1; Jim Albert1; Ryan Bell1; Dustin Mcrae1; Matt Colvin1; John T Kelly1; 1SRI International, Saint Petersburg, FL; 2Beaver 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 Miller1; Hunter Waite1; Tim Brockwell1; Paul Wilson2; John Hanley2; Ryan Blase2; John Roberts2; Keith Pickens2; Kelly Miller2; 1Southwest Research Institute, San Antonio, TX; 2Southwest 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 Virgen1; Sanjib Gurung2; David W. Murphy2; Benjamin D. Dubansky1; Guido F. Verbeck1; 1University of North Texas, Denton, TX; 2University of South Florida, Tampa, FL

**WP 335**

Field Induced Fragmentation Spectra of Volatile Organic Compounds with Reactive Stage Tandem Ion Mobility Spectrometry; Gary Eiceman1; Hossein Shokri1; Ben D Gardner2; 1New Mexico State University, Las Cruces, NM; 2Collins Aerospace, San Diemans, CA

**WP 336**

The Characterization of Ocean Realms and Life Signatures (CORALS) Prototype; Adrian Southard1; Lori Willhite2; Anais Bardyn2; Emanuel Hernandez2; Andrej Grubisic2; Ryan M. Danell2; Cynthia Gundersen2; Niko Minasola3; Alexander A. Makarov4; Christelle Braiso5; Ricardo Arevalo5; 1Universities Space Research Association, Greenbelt, MD; 2University of Maryland College Park, College Park, MD; 3NASA Goddard Space Flight Center, Greenbelt, MD; 4Danell Consulting, Inc., Winterville, NC; 5AMU Engineering, Inc., Miami, FL; 6Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 7CNRS UMR8038, Paris, France; 8University of Maryland, College Park, Maryland

**WP 338**

Single particle mass spectrometry with a colycoidal mass analyzer; Jason J Amsden1; Eleltra Piacentino1; Rafael Bento Serpa1; Charles B. Parker1; Yuri Zhilichev2; Roger P Sperline3; Robert Kingston4; Scott Tilden4; Justin Keogh4; Jeffrey T Glass1; M. Bonner Denton5; 1Duke University, Durham; 2Consultant, Durham, North Carolina; 3University 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 Cylcoidal Mass Analyzer; Raul Vyas1; Philip J. Herr1; Kathleen Horvath1; 1American University, Washington, DC; 2Academy of Sciences of the Czech Republic, Prague, Czech Republic; 3University of Colorado, Boulder, CO
WP 340
Title: Super-resolution in a cycloidal mass analyzer; Tanouir Aloui1; Raul Vyas2; Kathleen Horvath2; Charles B. Parker3; Rafael Bento Serpa4; Elettra Piacentino2; Maria Luisa Sartorelli1; Jennifer Stern1; Justin Keogh3; Robert Kingston4; Scott Tilden3; Roger P Spertine4; M. Bonner Denton5; Michael E. Gehm1; Jeffrey T Glass1; Jason J Amsden1; 1Duke University, Durham, NC; 2Broadway Analytical, LLC, Monmouth, IL; 3RTI International, Durham, NC; 4University of Arizona, Tucson, AZ

WP 341
Combined Atomic and Molecular (CAM) Ionization: The Diversity of the Liquid Sampling–Atmospheric Pressure Glow Discharge on a Compact Mass Spectrometer; Tyler J. Williams1; R. Kenneth Marcus1; Jacob R. Bills1; Jamey Jones2; 1Clemson University, Clemson, SC; 2Advion, Ithaca, NY

WP 342
Detection of Perfluoroalkyl and Polyluoroalkyl Substances through Automation of ASAP; Frank S. Yenchick1; Long Luo1; Sarah Trimpin1; 1Wayne State University, Detroit, MI

WP 343
Mechanism of Ionization Suppression from Ion Evaporation Model and a System for Real-Time Correction for Biological Samples; Thomas R Covey1; Andries P Bruins2; Chang Liu1; 1SCIEX, Concord, ON; 2University of Groningen, Groningen, Netherlands

WP 344
Efficient introduction of ionic compounds into LC-MS using the improved ESI unit; Application to dirty samples; Takanari Hattori1; Miho Kawashima1; Wataru Fukui1; Kazuo Mukaibatake1; 1Shimadzu Corporation, Kyoto, Japan

WP 345
Computer Assisted Development of 3D Printed Analytical Devices for Customized Open Port Probe-Electrospray Mass Spectrometry; Piotr Sosnowski1; Gérard Hopfgartner1; 1Life 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; Steve Bajic1; Claudi Black1; 1Waters Corporation, Wilmslow, United Kingdom

WP 347
Ion Dynamics Simulation Framework (IDSimF): An Open Source Trajectory Simulation Framework; Walter Wisssordt1; Duygu Ergodogu1; Marco Thinius1; Thorsten Benter1; 1University of Wuppertal, Wuppertal, Germany

WP 348
MALDI-2 laser post-ionization on a trapped ion mobility orthogonal time of flight instrument; Simeon Vens-Cappell1; Henning Peise1; Andreas Haase1; Aninka Koch1; Jens Hoehndorf1; 1Bruker Daltonik GmbH, Bremen, Germany

WP 349
Transport of Plasma generated Ions into a Fourier Transform Quadrupole Ion Trap using viscous gas flows; Chris Vico Heintz1; Yessica Brachthäuser1; Hendrik Kersten1; Thorsten Benter1; 1University of Wuppertal, Wuppertal, Germany; 2INFICON GmbH, Cologne, Germany

WP 350
High Sensitivity Analysis of Steroid Hormones with modified ESI to improve desolvation efficiency; Yuki Uno1; Yohei Toji1; Yusuke Inohana1; Tomoya Kudo1; Kazuo Mukaibatake1; 1Shimadzu 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. Attygalle1; Ramu Errabelli1; Julius Pavlov1; Isra Hassan1; Zhaoyu Zheng3; David Douce2; Steve Bajic1; 1Stevens Institute of Technology, Hoboken, NJ; 2Stevens Institute of Technology, Jersey City, NJ; 3Waters Corporation, Wilmslow, United Kingdom

WP 352
Hydrogen plasma based chemical ionization source for GC-MS; Steffen Bräcking1; Kai Kroll1; Hendrik Kersten1; Thorsten Benter1; 1University 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 Ehrlent1,2; Jan Heider2; Andreas Walte1; Ralf Zimmermann3,4; 1Photonion GmbH, Schwerin, Germany; 2University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; 3Heilmolholz 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; Gregory W. Vandergrift1,2; Erik T. Krogh1,2; Christopher G. Gill1,2,3,4; 1Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC; 2University of Victoria, Victoria, British Columbia; 3Simon Fraser University, Burnaby, BC; 4University of Washington, Seattle, WA
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**Acoustic Ejection Full Scan MS Analysis in Support of High Throughput Compound Plate QC:** Jun Zhang1; Yong Zhang2; Chang Liu3; Tom Covey4; Shu Li5; Harold Weller6; Wilson Shou7; 1Bristol-Myers Squibb, Lawrenceville, NJ; 2SCIEX, Concord, ON

WP 356  
**Development of High-Performance Capillary Vibrating Sharp-edge Spray Ionization (cVSSI) for Mass Spectrometry Analysis:** Chong Li1; Kushani Attanayake1; Stephen J. Valentine1; Peng Li1; 1West Virginia University, Morgantown, WV

WP 357  
**Native MS studies of proteins using capillary Vibrating Sharp-edge Spray Ionization (cVSSI):** Daud Sharif1; Samira Hajian Foroushani1; Kushani Attanayake1; Anthony Debastiani1; Chong Li1; Peng Li1; Stephen J Valentine1; 1West Virginia University, Morgantown, WV

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**Factors affecting ionization of small molecules by capillary vibrating sharp-edge spray ionization (cVSSI):** Kinkini Udara Jayasundara1; Anthony Debastiani1; Chong Li1; Daud Sharif1; Sara Macios1; Peng Li1; Stephen J Valentine1; 1West Virginia University, Morgantown, WV

WP 359  
**Velox Sample Cartridge with Snap-in Solid-Phase Extraction Column for Paper Spray Mass Spectrometry:** Chau Nguyen1; Nicholas Manicke2; 1Indiana University - Purdue University Indianapolis, Indianapolis, IN; 2Indiana University - Purdue University Indianapolis, Indianapolis, IN

WP 360  
**Advances in Automated Multi-ionization Mass Spectrometry:** ESI, SAI, MALDI: Khoa Hoang1; Milan Pophristic1; Sarah Trippin1, 2; Charles N McEwen1, 3; 1MSTM LLC, Newark, DE; 2Waters Corporation, Milford, MA; 3University of the Sciences in Philadelphia, Philadelphia, Pennsylvania

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**ION MOBILITY: APPLICATIONS I**

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**Ion/Ion Proton Transfer Reaction for Enhancing Peak Capacity in an Ion Mobility/Mass Spectrometry Bottom-up Proteomics Experiment:** Rebecca L Cain1; Ian Webb2; 1Indiana University Purdue University Indianapolis, Indianapolis, IN; 2Indiana 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 Nagy1; Isaac K. Atta1; Christopher R. Conant1; Weijing Liu1; Sandiya V. B. Garimella1; Harsha P. Guanawarden1a; Jared B. Shaw1; Richard D. Smith1; Yehia M. Ibrahim1; 1Pacific Northwest National Laboratory, Richland, WA; 2Johnson 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 King1, 2; Mark Ritchie2; Lee Gethings1; Lauren Mullin1; Robert Plumb3; Ian D Wilson4; 1Waters Corporation, Wilmslow, United Kingdom; 2Murdoch University, Perth, Australia; 3Waters Pacific Pte. Ltd., Singapore, Singapore; 4Waters Corporation, Milford, MA; 5Imperial 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 Girard1; Patrick Knight1; Roger Giles2; Gérard Hopfgartner1; 1Life Sciences Mass Spectrometry, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; 2Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom

WP 365  
**Application of Ion Mobility Specificity to Identify Food Additive Charged Isomers and Conformers:** Michael Mccullagh1; Severine Goscinny2; Kenneth Rosnack3; 1Waters Corporation, Wilmslow, United Kingdom; 2Sciensano, Brussels, Belgium; 3Waters Corporation, Milford, MA

WP 366  
**Structures for Lossless Ion Manipulation-MS for High Resolution, High Throughput Lipid Biomarker Analysis:** Kelly Wormwood1; Ravinder Earla1; James R. Arndt1; Liulin Deng1; Anisha Yadav1; Stephen Kruka1; Daniel Debord1; Laura Maxon1; Kim Ekroos2; 1MOBILion Systems Inc., Chadds Ford, PA; 2Lipidomics 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 Baker1; Pei Chen2; Jianghao Sun3; 1Waters, Inc., Pleasanton, CA; 2USDa-ARS, Beltsville, MD; 3USDa-ARS, Beltsville, MD

WP 368  
**DMS-MS for Rapid Characterization of Polysorbate 80 Samples:** Jay S. Bhano1; Nan Wang1; Alice Newman2; Bangping Xiang3; Li-Kang Zhang3; Kudrat Goswami1; Damon Barbacci2; Simon Hamilton2; Scott A. Mcluckey1; 1Purdue University, West Lafayette, IN; 2Merck & Co., Kenilworth, NJ

WP 369  
**Identification of Structural Isomers Utilizing a Deep Neural Network with a Metabolite-Specific Compound Library:** Maria V. Fawaz1; Ian S. McIntosh1; Xiang Yu1; Richard Gundersdorf1; Mark T. Cancilla1; 1Merck, 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. Butler1; Jaclyn Gowen
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**Deeper proteome coverage of musculoskeletal samples:**
- **Emma Doud**
- Xiaolong Zhong
- Joseph Rupert
- Matt Willett
- Shourjo Ghose
- Teresa Zimmers
- Amber L Moseley
- Indiana University School of Medicine, Indianapolis, IN
- Bruker Scientific LLC, Billerica, MA
- 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
- Dale A. Cooper-Shepherd
- Pavel V. Shliaha
- James I. Langridge
- Ole N. Jensen
- University of Southern Denmark, Odense M, Denmark
- Waters Corporation, Wilmington, United Kingdom

**WP 373**

**The Application of Ion Mobility-Mass Spectrometry towards Structural Characterization of α-Synuclein:**
- John M. Gordon
- Christopher S. Mallis
- David H. Russell
- Texas A&M University, College Station, TX

**WP 374**

**Towards native top-down sequence analysis of protein isoforms using tandem-trapped ion mobility spectrometry / mass spectrometry (Tandem-TIMS/MS):**
- Kirsten Tucker
- Mengqi Chai
- Fanny C Liu
- Christian Bleiholder
- Florida State University, Tallahassee, FL

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**Using SLIM-based ion mobility with on-board CID together with cryogenic ion spectroscopy for glycan analysis:**
- Priyanka Bansal
- Robert P. Pellegrinelli
- Vasily Yatsyna
- Ali Abi Khodr
- Stephan Warnke
- Ahmed Ben Faleh
- Eduardo Carrascosa
- Lei Yue
- Natalia Yalovenko
- Vicki H. Wysocki
- Thomas R. Rizzo
- Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland
- 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
- Mateusz Kozysztof Lacki
- Ute Distler
- Stephanie Kaspar-Schoenefeld
- Scarlet Koch
- Nadine Vewinger
- Claudia Paret
- Alex Henneman
- Joerg Faber
- Connie R. Jimenez
- Stefan Tenzer
- Medical Center of the Johannes Gutenberg University, Mainz, Germany
- Bruker Daltonic GmbH, Bremen, Germany
- Amsterdam AMC, Amsterdam, Netherlands

**WP 377**

**Ion Mobility Mass Spectrometry as an Efficient Tool for Identification of Streptorubin B in Streptomyces coelicolor M145:**
- Andrew P Marshall
- Andrew R Johnson
- Marvin M Vega
- Regan J Thompson
- Erin E Carlson
- University of Minnesota, Minneapolis, MN
- Indiana University, Bloomington, IN
- Northwestern University, Evanston, IL
- University of Minnesota, Minneapolis, MN
- University of Minnesota, Minneapolis, MN/55455

**WP 378**

**At-line profiling degradation products of peptide drug teriparadine by advanced robotics coupled with ion mobility mass spectrometry: A top-down approach:**
- Mack Shih
- Maxwell Korang-Yeboah
- Muhammad Azharaf
- Sau Lee
- Patrick Faustino
- Jinhui Zhang
- FDA, Silver Spring, MD

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**Advancing Data Independent Acquisition and Data Processing Strategies for IM-QTOFMS:**
- Max L. Feuerstein
- Ruwan T. Kuruluwage
- Hiroshi Tsuchiya
- Tim Caouss
- Stephan Hann
- University of Natural Resources and Life Sciences (BOKU), Vienna, Austria
- Agilent Technologies, Santa Clara, CA
- RIKEN Center for Sustainable Resource Science, Yokohama, Japan
- 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
- Johann Le Maître
- Mark E. Ridgeway
- Alfred P. Marshall
- Ralf Zimmermann
- Bruker Daltonik GmbH, Bremen, Germany
- Bruker Daltonics, Billerica, MA
- International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France
- Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany
- University of Rouen-Normandy, Mont Saint Aignan, France
- Total Refining and Chemicals, Harfleur, France
- Bruker Daltonics, Billerica, MA
- 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
- Drupad K Trivedi
- Eleanor Sinclair
- Sze Hway Lim
- Caitlin Walton-Doyle
- Kaneez Jafri
- Joy Milne
- Monty Silverdale
- Perdita E Barran
- University of Manchester, Manchester, United Kingdom

**WP 382**

**Rapid Chemical Description of Organic Aerosols with a Direct Inlet Coupled to Trapped Mobility Time-of-Flight Mass Spectrometry:**
- Lukas Friederici
- Christopher Paul Rüger
- Janné Jänis
- Christian Albers
- Heino M. Heyman
- Ralf Zimmermann
- University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany
- University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany
- University of Eastern Finland, Joensuu, Finland
- Bruker Daltonik GmbH, Bremen, Germany
- Bruker Scientific LLC, Billerica, MA
- 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
- Gustavo de Albuquerque Cavalcanti
- Monica C. Padilha
- Katrina L. Leaptrot
- Nadjali A. Chung
- Jody C. May
- John A. McLean
- Henrique M. Pereira
- Department of
Multiplexed IR spectroscopy of ion-mobility separated glycans using Hadamard transform; Vasyl Yatsyna¹,²; Ali H Abikhodr¹; Thomas R. Rizzo¹; ¹EPFL/LCPM, Lausanne, Switzerland; ²University of Gothenburg, Gothenburg, Sweden

The Paternó-Büchi Reaction as a Method for Improved Ion Mobility Separation of Isomeric Steroids; Stine S. H. Olsen¹; Samuel W Maddox¹; Diane C Velosa¹; Aurora Burkus-Matesevac¹; Christopher D. Chouinard¹; ¹Florida Institute of Technology, Melbourne, FL
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10 min LC-MSMS analysis of fatty acids in triacylglycerols to compare human serum and food; Doriane Toinon1; Yamada Masaki1; Shimadzu corporation, Kyoto, Japan

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Systematic Approach to Method Development for Lipomics Analysis of Biological Samples Using Trend Analysis and Lipostar; Rachelle Golden1; Laura Goracci2; Paolo Tiberi3; Gabriele Cruciani3; Liu Guo1; Alla Kloss1; Sanofi, Vitry Sur Seine, France; University of Perugia, Perugia, Italy; Molecular Discovery, Ltd., Borehamwood, United Kingdom

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Untargeted lipidomic analysis of human retinas using LC-MS/MS and MALDI imaging mass spectrometry; Anika Kothari1,2; David M Anderson1; Jarad A. Fincher1; Nathan Heath Patterson1; Lee S Cantrell1; Jeffrey D. Messinger1; Christine A. Curcio1; Kevin L. Schey1; Department of Biochemistry, Vanderbilt University, Nashville, TN; Department of Ophthalmology and Visual Sciences, University of Alabama at Birmingham, Birmingham, AL

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Serum lipid profiling from a randomized trial on the effects of dietary patterns on obesity; Sunhee Jung1; Ji-Hee Shin1; Seoyoung Jang1,3; Dong-Mi Shin1; Geum-Sook Hwang1,3; Korea Basic Science Institute, Seoul, South Korea; Seoul National University, Seoul, South Korea; Ewha Womans University, Seoul, South Korea; Seoul National University, Seoul, South Korea

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Lithium ion addition-based UPLC-MS/MS analysis of multi-class ketolic steroid hormones containing a 3-hydroxy group; Qiuyi Wang1; Kimiko Shimizu2; Kanako Maehata2; Yue Pan1; Koki Sakurai1; Takatoshi Hikida1; Yoshitaka Fukada2; Toshihumi Takao1; Osaka University, Suita, Japan; The University of Tokyo, Tokyo, Japan

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Oncofinder: a novel platform for screening benign nevi from melanomas based on lipid phenotype using mass spectrometry and machine learning; Roberto A. Fernández Regueira1; Egoitz Astigarraga1; José A. Fernández2; Dolores Boyano1; Aintzane Asumendi2; Michael N. Nairn3; Shaukat Ibrahim3; Simona Salivo5; Matthew E. Openshaw3; Gabriel Barreda-Gómez1; IMG Pharma Biotech S.L., Derio, Spain; University of the Basque Country (UPV/EHU), Barrio Sarriena, Spain; Shimadzu, Manchester, United Kingdom

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AMP-activated protein kinase activation inhibits ferroptosis through PUFA metabolism; Fereshteh Zandkarimi1; Hyemin Lee2; Boyi Gan3; Brent R. Stockwell4; Columbia University, New York, NY; University of Texas MD Anderson Cancer Center, Houston, TX

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Infusion MS/MSALL with Differential Mobility Separation : A High-throughput Lipidomic Solution for Untargeted Profiling; Mackenzie Pearson1; Paul Norris2; Santosh Kapil2; Darren Dumiao4; Sciex, Redwood City, CA; Sciex, Framingham, MA; SCIEX, Redwood Shores, California 1201

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Hight throughput lipidomics for bacterial phenotyping; Rutan Zhang1; Nate K. Ashford2; Amy Li3; Dylan H. Ross2; Brian J. Werth2; Libin Xu2; University of Washington, Seattle, WA; University of Washington, Seattle, WA
WP 404  Analysis of Stable Isotope Labeled N-docosahexaenoylphosphatidylethanolamine Molecular Species Distribution in Neuronal Cell Culture; Karl R Kevala1; Michel Lagarde2; Arthur Spector3; Hee-Yong Kim1; 1National Institutes of Health, Rockville, MD; 2Universite 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 Veillon1; Marc Warmoes1; Abdul Wadud Khan1; Reetakshi Arora1; Jennifer Wargo1; John N Weinstein1; Philip L Lorenzi1; 1MD Anderson Cancer Center, Houston, TX

WP 407  Alterations in mouse brain lipidome during neurodevelopment and in a model of Smith-Lemli-Opitz syndrome; Amy Li1; Kelly M Hines1; 2Libin Xu1; 3University of Washington, Seattle, WA; 4University of Georgia, Athens, GA

WP 408  Lipidomic analysis of plasma from patients with cervical cancer and cervical intraepithelial neoplasia using LC-MS approach; Seoyoung Jang1; Miso Nam1; Sunhee Jung1; Mi Kyung Kim2; Geum-Sook Hwang1; 1Korea Basic Science Institute, Seoul, South Korea; 2National Cancer Center, Goyang-si, South Korea

WP 409  Untargeted lipidomics of viral particles and cell lysates following vesicular stomatitis virus infection; Katherine E. Havranek1; Melinda A. Brindley1; Kelly M Hines1; 1University of Georgia, Athens, GA

WP 410  Unequivocal mapping of ether lipids by LC-MS/MS by using plasmalogen-deficient mouse tissues; Jakob Koch1; Katharina Lackner1; Yvonne Wohlfarter1; Sabrina Sailler1; Johannes Zschocke1; Katrin Watschinger2; Markus Keller1; 1Institute of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; 2Institute 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 Lee1; Jeeyoun Jung1; 1Korea 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 Yazd1; Vanessa Y. Rubio1; Richard A. Yost1; Timothy J. Garrett1; 1University 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. Kemperman1; Chris W.W. Beecher2; Timothy J. Garrett1; Richard A. Yost1; 1University of Florida, Gainesville, FL; 2IROA 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 Zhang1; 2; Dinesh K. Barupal1; Sili Fan1; Oliver Fiehn1; 1West Coast Metabolomics Center, UC Davis, Davis, CA; 2Department of Chemistry, University of California, Davis, Davis, CA

WP 416  Inter-laboratory comparison of metabolite measurements for metabolomics data integration; Yoshihiro Izumi1; Fumio Matsuda2; Akiyoshi Hirayama3; Kazutaka Ikeda4; Yoshihiro Kita5; Kanta Horie6; Daisuke Saigusa7; Kosuke Saito8; Yuji Sawada9; Hiroki Nakanishi10; Nobuyuki Okahashi2; Masatomo Takahashi1; Motonao Nakao1; Kosuke Hata1; Yutaro Hoshi11; Motohiko Morihara12; Takeshi Bamba1; Yoshiya Oda13; 1Korea Institute of Oriental Medicine, Daejeon, South Korea; 2Graduate School of Information Science and Technology, Osaka University, Osaka, Japan; 3Institute for Advanced Biosciences, Keio University, Yamagata, Japan; 4Kazusa DNA Research Institute, Chiba, Japan; 5Graduate School of Medicine, The University of Tokyo, Tokyo, Japan; 6Division of Medical Safety Science, National Institute of Health Science, Kanagawa, Japan; 7Graduate School of Health Science, Kanagawa, Japan; 8Riken Center for Sustainable Resource Science, Kanagawa, Japan; 9Research Center for Biosignal, Akita University, Akita, Japan; 10Pharmacokinetic Research Laboratories, Ono Pharmaceutical Co., Ltd., Ibaraki, Japan; 11Translational Research Laboratories, Ono Pharmaceutical Co., Ltd., Osaka, Japan; 12Medical 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 Schneider1; John Janiszewski2; Sam Michael1; Matt Hall1; Stephen Ferguson1; Michael Iannotti1; Surbhi Poddar1; Maheswari Karthikeyan2; Sunil Dhakad3; Raghav Sehgal4; Rebecca Cardone3; Qiushi Sun3; Richard G. Kibbey3; Jackson Strowbridge3; Aiko Barsch3; Allan R Brasier1; Michelle Kimple1; Ying Ge1; 1University of Wisconsin-Madison, Madison, Wisconsin; 2Bruker Daltonics, Billerica, MA; 3Bruker Daltonics, Bremen, Germany

WP 418  Untargeted FTICR-MS Based Plasma Metabolomic Analysis and Translation to Type 2 Diabetes; Yanlong Zhu1; Benjamin Wancewicz2; Michael Schaid1; Kent Wenger1; Yutong Jin1; Heino M. Heyman2; Christopher Thompson2; Aiko Barsch3; Allan R Brasier1; Michelle Kimple1; Ying Ge1; 1University of Wisconsin-Madison, Madison, Wisconsin; 2Bruker Daltonics, Billerica, MA; 3Bruker 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; Lars M. Blank; 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; Subramaniam Pennathur; Anna Mathew; University of Michigan, Ann Arbor, MI; University of Michigan Medical School, BRFC Metabolomics Core, Ann Arbor, Michigan; University of Michigan, Ann Arbor, MI

WP 421 High Performance Chemical Isotope Labeling (HP-CIL) LC-MS Platform for High-Coverage Quantitative Metabolomics; Shuang Zhao; University of Alberta, Edmonton, AB; 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; Akane Murayama; Takaharu Hattori; Jun Watanabe; Shimadzu Corporation, Global Application Development Center, Kyoto, Japan; Shimadzu Corporation, MS Business Unit, Kyoto, Japan

WP 423 Single egg metabolomics as the latest tool in the Drosophila Melanogaster toolbox; Ryan D Sheldon; Eduardo Perez-Mojica; Ellen Griggs; Christine Isaguirre; Abigail Ellis; Brejnev M. Muhire; Russeil G. Jones; Adelheid Lempradl; 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; Kazuyuki Kasahara; Laura-Isobel McCaill; University of Oklahoma, Dept. of Chem & Biochem, Norman, Oklahoma; Laboratories of Molecular Anthropology and Microbiome Research, University of Oklahoma, Norman, OK; Department of Bacteriology University of Wisconsin-Madison, Madison, Wisconsin; Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; 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; Hongxia Wang; Xueqing Zhao; Haibo Qiu; Ning Li; Regeneron Pharmaceuticals Inc., Tarrytown, NY

WP 426 Metabolic rewiring of cardiomyocytes after acute infection of Trypanosoma cruzi; Gabriela Venturini; Juliana Alvim; Kallyandra Patinha; Karina Cardozo; Valdemir Carvalho; Jose Eduardo Krieger; Jonathan Seidman; Christine Seidman; Alexandre Pereira; Harvard Medical School, Boston, MA; Heart Institute, Medical School, USP, Sao Paulo, Brazil; Fleury Group, Sao Paulo, Brazil; Brigham and Women's Hospital, Boston, MA

WP 427 Elucidating unknown pathways in Plasmodium falciparum with labeled metabolomics; Conor Jenkins; Ioanna Nta; Amanda Souza; Benjamin Orsbum; Hood College, Frederick, MD; Proteomic Und Genomic Sciences, Glen Rock, PA; Thermo Fisher Scientific, San Jose, California; University of Virginia School of Medicine, Charlottesville, VA

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WP 428 Studying Neural Tissue Formation by Analyzing Neural-Tissue Fated Cell Clones from Developing X. laevis Embryos using LC-HRMS; Jie Li; Peter Nemes; 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; Eiquan Fan; Niusheng Xu; Thermo Fisher Scientific, Shanghai, China

WP 430 Elucidation of carotenoids in microalgae formulations by ultra-high resolution mass spectrometry combined with APCI; Eduardo Sommella; Emanuela Salvati; Giulio Maria Conte; Matthias Witt; Pietro Campiglio; University of Salerno, Fisciano, Italy; 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; Emanuela Salvati; Matthias Witt; Christopher Thompson; Pietro Campiglio; University of Salerno, Fisciano, Italy; Bruker Daltonik GmbH, Bremen, Germany; Bruker Daltonics, Billerica, MA

WP 432 Untargeted Lipidomics Analysis of Plasma Samples from Dyslipidemic Patients; Anna Maria Alves De Piloto Fernandes; Gustavo Henrique Bueno Duarte; Alex Aparecido Rosini Silva; Joyce Aparecida Barreto; Márcia Aparecida Antonio; Andréa de Melo Porcar; Patricia de Oliveira Carvalho; Universidade São Francisco, Bragança Paulista, Brazil; Universidade Estadual de Campinas, Campinas, Brazil; 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; Mark B. Meads; Dario M. Magaletti; Joy D. Guingab-Cagmat; Paula S.
WP 435  Five Easy Metrics of Data Quality for LC-MS Based Global Metabolomics; Daniel Raftery1; Xinyu Zhang2; Jiyang Dong3; 1UW Medicine, SLU, Seattle, WA; 2University of Washington, Seattle, WA; 3Xiamen 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 Helling1; Gordon Custer2; Linda Van Diepen3; Franco Basile1; 1Department of Chemistry, University of Wyoming, Laramie, Wyoming; 2Department 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 Chilakala1; Carly Strelez2; Ah Young Yoon1; Shannon Mumenthaler3; Jonathan E Katz1; 1Lawrence 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; Garthia Pacheco1; Daniel Morris2; Christopher Ziegler2; Joao Gomes2; Leah P Shriver2; 1University of Akron, Akron, OH 44325; 2University of Akron, Akron, OH; 3Cleveland Clinic, Cleveland, OH 44195

WP 439  Metabolomics approach reveals dysbiosis in the gut microbiota by Salmonella infection; Yongseok Kim1; Maryam Baniasad1; Anice Sabag-Daigle1; Michael T. Shaffer2; Kelly C. Wrighton2; Brian M.M. Ahmer1; Vicki H Wysocki1; 1The Ohio State University, Columbus, OH; 2Colorado State University, Fort Collins, CO

WP 440  High Resolution Mass Spectrometry Characterization of Essential Oil and Extractives from Norway Spruce buds; Omolara Mofikoya1; Marko Mäkinen1; Janne Jänis1; 1University of Eastern Finland, Joensuu, Finland

WP 441  Getting the most out of GC-HRMS data using novel R-based software tools; Carsten Jaeger1; Jan Liseč1; 1Federal Institute for Material Research and Testing, Berlin, Germany

WP 442  Metabolomics study of klk8 deficient mouse with different instruments and ionization/detection methods; Lukaš Kucera1; Ashkan Zareie1; Kryštof Klima1; Vendula Novosadová1; Matthias Witt2; Heino Heyman3; Radislav Sedláček1; 1Czech Centre for Phenogenomics, Prague, Czech Republic; 2Bruker Daltonik GmbH, Bremen, Germany; 3Bruker 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 Ehler1; Christopher Aboo1; Verena Tellstroem2; Mette Hedegaard Thomsen1; Allan Stensballe1; 1Aalborg University, Aalborg, Denmark; 2Bruker Daltonik GmbH, Bremen, Germany

WP 444  Untargeted UHLC-HR-QTOF-MS metabolomics study to unravel metabolites controlling wood formation in aspen trees; Maodaline A. Reinkensmeier1; Ilara G.F. Budzinski2; Thomas Moritz3; 1Bruker Daltonics, Bremen, Germany; 2Umeå Plant Science Centre, Department of Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; 3Swedish Metabolomics Centre, Swedish University of Agricultural Sciences, Umeå, Sweden; 4Novo 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 Gamisjua1; 2Chupalav Eldarov1; 3Vitaliy Chagovets1; Luiza Ibragimova1; Veronika Smolíková1; Elena Kalinina1; Victor Zgoda1; Mikhail Bobrov1; 1National Medical Research Center for Obstetrics, Gynecology and Perinatology, Moscow, Russia; 2Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, RAS, Moscow, Russia; 3Belozersky Institute Of Physico-Chemical Biology, Moscow, Russia; 4Institute 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 Davis1; Peter Sullivan1; Steven Kurina1; Joanna E. Burdette1; Jimmy Orjala1; 1College 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 Miguez1; Mark Styczynski1; 1Georgia 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 Zhang1; Thomas Rydzak2; Ryan A Groves2; 1Independent Researcher, Calgary, AB; 2University of Calgary, Calgary, AB

WP 449  Expanding the detection and discovery of ribonucleoside modifications by higher-energy collisional dissociation mass spectrometry (HCD-MS); Manasses Jora1; Peter A. Lobue1; Robert L. Ross1; Ningxi Yu1; 1Independent Researcher, Calgary, AB
**WP 450**
Use of Ion-Mobility Mass Spectrometry to Determine Fluoroalcohol-induced Alterations in the Secondary Structure of Oligonucleotides; J. Michael Sutton; Michael G Bartlett; University of Georgia, Athens, GA

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Ultrasonic determination of rare modified nucleotides based on novel hydrazine labelling reagents; Yue Yu; Fang Yuan; Xin Zheng; Qing-Cui; Yingling Zhou; Xin-Xiang Zhang; Peking University, Beijing, China; Union Medical College Hospital, Beijing, China; Peking University, Haidian, China

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Oligonucleotide Analysis via Microchip CE-MS; Ashley Bell; Erin A Redman; J. Scott Mellors; 908 Devices, Inc., Carrboro, NC

**WP 453**
Use of Ion-Mobility Mass Spectrometry to Determine Fluoroalcohol-induced Alterations in the Secondary Structure of Oligonucleotides; J. Michael Sutton; Michael G Bartlett; University of Georgia, Athens, GA

**WP 454**
Stable isotopes labeling with nucleosides in cell culture as an approach to RNA modification dynamics; Mayu Tsuchiya; Yuko Nobe; Yuka Yamaki; Yoshio Yamauchi; Hiroshi Nakayama; Masato Taoka; Tokyo Metropolitan University, Hachioji, Japan; RIKEN Center for Sustainable Resource Science, Wako, Japan

**WP 455**
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**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; Tracy Hodges; Laura Snyder; Sarah C. Keane; University of Michigan, Ann Arbor, MI; University of Michigan, Ann Arbor, MI

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Characterization of phosphate- and phosphorothioate-linked nucleic acids by 213-nm ultraviolet photodissociation tandem mass spectrometry; Hiroshi Nakayama; Daihuke Higo; Masami Koike; Masato Taoka; RIKEN CSRS, Wako, Japan; Thermo Fisher Scientific, Yokohama, Japan; Tokyo Metropolitan University, Hachioji, Japan

**WP 458**
Characterization of phosphate- and phosphorothioate-linked nucleic acids by 213-nm ultraviolet photodissociation tandem mass spectrometry; Hiroshi Nakayama; Daihuke Higo; Masami Koike; Masato Taoka; RIKEN CSRS, Wako, Japan; Thermo Fisher Scientific, Yokohama, Japan; Tokyo Metropolitan University, Hachioji, Japan

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**WP 460**
Recent advances in mass spectrometry of oligonucleotides; Michael G. Bartlett; J. Michael Sutton; Vidya Annavarapu; Guillerme Jendroba Guimaeras; University of Georgia, Athens, GA

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Diel-based HILIC Chromatography and HRAM Mass Spectrometry for the Analysis of Double-stranded Oligodeoxynucleotides Crosslinked by the Bacterial Genotoxin Colibactin; Alessia Stornetta; Peter W. Villalta; Erik S. Carlson; Emily P. Balskus; Silvia Balbo; University of Minnesota Masonic Cancer Center, Minneapolis, MN; Department of Chemistry and Chemical Biology, Harvard University, Boston, MA; Division of Environmental Health Sciences, University of Minnesota, Minneapolis, MN

**WP 462**
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**WP 464**
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Facile determination of phosphorylation sites in peptides using two-dimensional mass spectrometry and UVPD; Johanna Paris; Tomos E Morgan; Alina Theisen; Bryan P. Marzullo; Anisha Haris; Christopher A. Wootton; Mark P. Barrow; John O’hara; Peter B O’Connor; University of Warwick, Coventry, United Kingdom; UCB, Slough, United Kingdom
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N-Glycan Profiling Using RapiFluor-MS N-Glycan Kit in Biopharmaceutical Discovery and Development; Yanyan Lu¹; Ying Zhou¹; ¹Alkermes, Inc, Waltham, MA

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A holistic approach to comprehending the in vivo intact stability of novel modalities using LC-MS and capillary electrophoresis-based methods; Hannah Chi¹; Cong Wu¹; Phillip Chu¹; Hilda Hernandez-Barró¹; William Sawyer¹; Neha Srikumar²; Brian Roper³; Thomas Niedringerhaus¹; Adrian Papas³; John Tran¹; ¹Genentech, South San Francisco, CA; ²University of Pennsylvania, Philadelphia, PA; ³ProteinSimple, San Jose, California

**WP 474**
Automated Workflow for Quantification of Intact Monoclonal Antibodies by CEX-MS; Angela Criscuolo¹; Marc Guender²; Sara Carillo³; Florian Füssli⁴; Ken Cook⁴; Jonathan Bones³; ¹Thermo Fisher Scientific, Dreieich, Germany; ²Thermo Fisher Scientific, reinach, Switzerland; ³National Institute of Bioprocessing Research and Training, Dublin, Ireland; ⁴Thermo Fisher Scientific, Hemel, United Kingdom

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Enhanced Detection of Host Cell Proteins enabled by use of Collisonal Cross Sections; Stuart Pengelley¹; Christine Paul²; Eckhard Belau¹; Waltraud Evers¹; Tim Welsink¹; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²InVivo BioTech Services, Henningsdorf, Germany

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**WP 477**
Meeting the Challenges of Implementing the Multi-Attribute Method (MAM) in Regulated/Non-Regulated Environments; Nilini Ranbaduge¹; Ying Qing Yu²; Weibin Chen¹; ¹Waters Corporation, Milford, MA; ²Waters Corps, Milford, MA

**WP 478**
Parallel Reaction Monitoring (PRM) Quantification of Herceptin and Trastuzumab N-Glycans; Joshua Shipman¹; Jason Rodriguez¹; Connie Ruzicka²; David Keir¹; Kang Chen¹; Hongbin Zhu¹; ¹Division of Complex Drug Analysis, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO; ²Division 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; Maurizio Bronzetti¹; Jonathan Jones²; Peter Haberl³; Catherine Evans⁴; ¹Genedata Inc, San Francisco, CA; ²Genedata Ltd, Cambridge, United Kingdom; ³Genedata GmbH, Munich, Germany; ⁴Genedata AG, Basel, Switzerland

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Integrated characterization and screening workflows to simplify the design of MAM methods; Guillaume Tremintin¹; Detlev Suckau²; Yue Ju¹; Anjali Alving³; ¹Bruker Daltonics, San Jose, CA; ²Bruker Daltonics GmbH, Bremen, Germany; ³ProteinSimple, Billerica, MA

**WP 481**
Highly sensitive LC-MS/MS workflow for targeted quantification of host cell proteins; Lei Xiong¹; Yi Zhang¹; Ian Moore²; ¹SCIEX, Redwood Shores, CA; ²SCIEX, Concord, ON

**WP 482**
A Fast and Simple Immuno-mass Spectrometry Based Method Enables Universal Preclinical Bioanalysis for IgG-1 Type mAb; Jiahuu Tang¹; Yue Zhou¹; ¹Thermo Fisher Scientific, Shanghai, China, shanghai, China
WP 484 **Understanding the Proteomic Differences Between Primary and Super-charged Natural Killer Cells;** Lucy Wanrong Gao1; Meng-Wei Ko2; Anahid Jewett2, 3; Julian Whitelegge1; 1The Pasarow Mass Spectrometry Laboratory, The Jane and Terry Semel Institute for Neuroscience and Human Behavior, David Geffen School of Medicine, UCLA, Los Angeles, CA; 2Division of Oral Biology and Oral Medicine, The Jane and Jerry Weintraub Center for Reconstructive Biotechnology, UCLA, Los Angeles, CA; 3The 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 Upadhyay1; Jeffrey Savas1; 1Northwestern University, Chicago, IL

WP 486 **A universal LCMS workflow for therapeutic monoclonal antibody bioanalysis;** Li Sun1; Lisa O’callaghan1; Daniel Spellman1; 1PPDM Bioanalytics, Merck & Co., Inc., West Point, PA

WP 487 **LC-MS/MS method development of aflibercept using Fab-selective proteolysis nSMOL technology;** Nozomi Maeshima1; Kenichi Aizawa2; Manami Kobayashi1; Kota Ishioka1; Takashi Shimada1; Junichi Masuda1; 1Shimadzu Corporation, Hadano, Japan; 2Jichi Medical University, Shimotsuke, Japan; 3Shimadzu Scientific Instruments, Bothell, WA

WP 488 **Bioanalytical Strategies for Comprehensive Pharmacokinetic and Catabolism Assessments of ADCs, A Case Study with MEDI3726;** Eric Ma1; Michael P Waldron1; Markling Pey1; Moucun Yuan1; Omnia Ismaiel1; William R. Mylott2; Yue Huang2; Christopher Del Nagro2; Kemal Balic2; Meina Liang2; Lorin Roskos2; Anton I Rosenbaum2; 1PPD Laboratories, Richmond, VA; 2Clinical Pharmacology & Quantitative Pharmacology, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, 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 Xue1; Jie Pu1; Yang Liu1; Jun Qu1, 2; 1University at Buffalo, Buffalo, NY; 2New 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 Shi1; Brendan Powers1; David Good1; Shashank Gortyala1; Zachariah Herendeen1; Yongle Pang1; Aaron Ledvina1; Stephanie Cape1; Covance, Madison, WI

WP 491 **Comprehensive Investigation of Drug-Drug Conjugates Induced Ocular Toxicity Using Novel LC-MS-based Strategies;** Xiaoyu Zhu1; Min Ma1, 2; Ming Zhang1; Bo An1; Shihan Huo1; Yang Qu1; Jie Pu1; Jun Qu1, 3; 1University at Buffalo, Buffalo, NY; 2Roswell Park Comprehensive Cancer Institute, Buffalo, NY; 3New 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 Yang1, 2; Chao Xue1, 2; Ming Zhang1, 2; Yang Qu1, 2; Jun Qu1, 2; 1University at Buffalo, Buffalo, NY; 2Center 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 Huo1; Jie Pu1; Qingqing Shen1; Ming Zhang1, 2; Xiaoyu Zhu1; Jun Qu1, 2; 1University at Buffalo, Buffalo, NY; 2New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY

**PROTEINS: PTMS II**

WP 494 **CobB serves as a lysine de-2-hydroxyisobutyrylation 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-Paulet1; David Bouyssié2; Carine Froment2; Odile Burlet-Schiltz2; Lars J Jensen1; 1Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; 2Institut 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 Mathay1; Juan D. Chavez1; Jimmy K Eng1; James E Bruce1; 1University of Washington, Seattle, WA

WP 497 **A quantitative proteomics approach to investigate processes related to mitophagy in human cells;** Katharina Zittlau1; Anna Lechado-Terradas2; Sven Geisler3; Nicolas Nalpas1; Philipp Kahle3; Boris Macek1; 1Quantitative Proteomics and Proteome Center Tuebingen, Interfaculty Institute for Cell Biology, University of Tuebingen, Auf der Morgenstelle 15, Tuebingen, Germany; 2Functional Neurogenetics Department of Neurodegeneration, Hertie Institute for Clinical Brain Research and German Center for Neurodegenerative Diseases, Faculty of Medicine, University of Tuebingen Offried-Müller-Strasse 27, Tuebingen, Germany; 3Functional Neurogenetics Department of Neurodegeneration, Hertie Institute for Clinical Brain Research and German Center for Neurodegenerative Diseases, Faculty of Medicine, University of Tübingen Offried-Müller-Strasse 27, Tuebingen, Germany

WP 498 **Rapid assessment of protein structural heterogeneity using native LC/MS;** Wenhua Yang1; Igor A Kaltashov1; 1Univ. of Massachusetts/Chemistry Dept., Amherst, MA
WP 499  Identifying novel upstream kinases of the microtubule-associated protein Tau using fluorescence complementation mass spectrometry (FCMS); Der-Shyang Kao; Yanyan Du; W. Andy Tao; 1Purdue University, West Lafayette, IN; 2Purdue University, West Lafayette

WP 500  Mining the Proteome for Sulfenic Acid Modifications with Cell permeable clickable trans-cyclooctenol (TCOI) chemical probes; Uthpala I Seneviratne; 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; Bethany C. Taylor; Amanda L. Wong; Matthew V. Holt; Tao Wang; Nicolas L. Young; 1Baylor College of Medicine, Houston, TX

WP 502  Understanding the effect of nutrients on the epigenome; Arabella L Garcia; Peder J Lund; Benjamin A Garcia; 1Strath Haven High School, Wallingford, PA; 2University 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; Jun Zhu; Chen Bu; Xianming Liu; Ning Chen; Conor Mulliens; Heiner Koch; 1Bruker Daltonics, Shanghai, China; 2PTM Biolabs Inc., Hangzhou, China; 3Bruker Daltonics, Beijing, China; 4Bruker Daltonics, Billerica, MA; 5Bruker Daltonic GmbH, Bremen, Germany

WP 505  PhoSSPAir: An online deep learning-based tool to mine literature information on phosphorylation sites; Sara R. Savage; Yaoyun Zhang; Eric J Jaehnig; Hua Xu; Bing Zhang; 1Baylor College of Medicine, Houston, TX; 2Melax Technologies, Houston, TX

WP 506  Reconstructing Protein Charge Heterogeneity from a Bottom-Up Approach; Andrew Mahan; Bo Zhai; Robert Hepler; Andrew Nichols; Yong Joo Kim; Eric Carlson; Hirsh Nanda; 1Janssen R&D LLC., Spring House, PA; 2Protein Metrics, Cupertino, CA

WP 507  Highly Sensitivity Lysine Acetylation Profiling with Trapped Ion Mobility Spectrometry and PASEF; Xianming Liu; Jun Zhu; Chen Bu; Ning Chen; Xiaoxian Du; Shourio Ghose; Heiner Koch; 1Bruker Daltonics, Shanghai, China; 2PTM Biolabs Inc., Hangzhou, China; 3Bruker Daltonics, Beijing, China; 4Bruker Scientific LLC, Billerica, MA; 5Bruker Daltonics, Bremen, Germany

WP 508  Investigation of PTM changes in blood plasma proteome associated with AD and MCI; Maria Indykina; Natalia Zakharova; Anna Bugrova; Alexander Brzhozovskiy; Yana B. Fedorova; Svetlana I. Gavrilova; Allexey Kononikhin; Eugene (evgeny) Nikolaev; 1Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; 2Moscow Institute of Physics and Technology, Dolgoprudny, Russia; 3Skolkovo Institute of Science and Technology, Moscow, Russia; 4Mental Health Research Center, Russian Academy of Science, Moscow, Russia

WP 509  Sheepless Capillary Electrophoresis Coupled to Mass Spectrometry for Biopharmaceutical Characterization; Ruinan Yang; Gordon Nicol; Chenhua Zhang; Qiling Tang; Jie Ding; 1PPD, Middleton, WI

WP 510  Label-free quantification for top-down two-dimensional mass spectrometry; Matthias Halper; Marc-André Delsuc; Kathrin Breuiker; Maria Van Agthoven; 1University of Innsbruck, Institute of Organic Chemistry, Innsbruck, Austria; 2Institut de Génétique et de Biologie Moléculaire et Cellulaire, Illkirch-Graffenstaden, France; 3CASC4DE, Strasbourg, France

WP 511  Proteomic and Phosphoproteomic Profiling of Praziquantel Treatment on Schistosoma mekongi for Investigation of Potential Parasiticidal Mechanisms; Peerut Chienwichai; Poom Adisakwattana; Tipparat Thiangtrongtip; Yanin Limpanont; Sumate Ampawong; Onrapak Reamtong; 1Faculty of Medicine and Public Health, HRH Princess Chulabhorn Woman’s Medical College, Chulabhorn Royal Academy, Bangkok, Thailand; 2Department of Helminthology, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 3Department of Molecular Tropical Medicine and Genetics, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 4Department of Social and Environmental Medicine, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 5Department 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; Kwidna E. M. Opuni; Cornelia Koy; Bright Danquah; Maren Reepmeyer; Manuela Ruß; Peter Lorenz; Matthias Halper; Peder J Lund; Benjamin A Garcia; 1Faculty of Medicine and Public Health, HRH Princess Chulabhorn Woman’s Medical College, Chulabhorn Royal Academy, Bangkok, Thailand; 2Department of Helminthology, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 3Department of Molecular Tropical Medicine and Genetics, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 4Department of Social and Environmental Medicine, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand; 5Department of Tropical Pathology, Faculty of Tropical Medicine, Mahidol University, Ratchathewi, Thailand

WP 513  Saving millions of lives with 50,000 quantified proteomes of bacterial pathogens; Annegret Ulke-Lemee; Jenna Poelzer; Mario Valdez Tresanco; Soren Wacker; Thomas Rydzak; Sergei Noskov; Ian Andrew Lewis; 1University of Calgary, Calgary, AB
WP 514 Proteogenomics towards the characterization of antimicrobial peptide resistance patterns in Escherichia coli; Patric W. Sadecki; Leslie M. Hicks; UNC - Chapel Hill, Chapel Hill, NC

WP 515 Bottom-up Proteomics Reveals the Impact of Salmonella Infection on the Gut Environment; Maryam Baniasad; Yongseok Kim; Anice Sabag-Daigle; Michael T. Shaffer; Kelly C. Wrighton; Brian M.M. Ahmer; Vicki H. Wysocki; The Ohio State University, Columbus, OH; Colorado State University, Fort Collins, CO

WP 516 Limited Tryptic-Isotope Digestion Dilution Mass Spectrometry (LTD-IDMS): A regent-free analytical assay to quantify hemagglutinin of H5N1 influenza vaccine material; Hans C Cooper; Yuhong Xie; William Sutton; Giuseppe Palladino; John R Barr; Ethan C. Settembre; Yingxia Wen; Tracie Williams; Centers of Disease Control and Prevention (CDC), Atlanta, GA; Sequis, Cambridge, MA 02139

WP 517 Proteomic approaches for the epidemiology and diagnosis of tick-borne diseases; Paola Cantero; Pierre Boyer; Josiane Saade; Nathalie Boulanger; Benoît Jaulhac; Maria Kazimirova; José De La Fuente; Marie Jalovecova; Laurence Ehret-Sabatier; Laboratoire de Spectrométrie de Masse BioOrganique, UMR 7178, CNRS, Université de Strasbourg, Strasbourg, France; 2UR729, Virulence bactérienne précoce: groupe Borrelia, Fédération de Médecine Translationnelle de Strasbourg, Université de Strasbourg, Strasbourg, France; 3Institute of Zoology, Slovak Academy of Sciences, Bratislava, Slovakia; 4SaBio, IREC, Ronda de Toledo s/n, Ciudad Real, Spain; 5Department of Veterinary Pathobiology, Center for Veterinary Health Sciences, Oklahoma State University, Stillwater, Oklahoma; 6Institute of Parasitology, Biology Centre of the Czech Academy of Sciences, Ceske Budejovice, Czech Republic; 7Faculty 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; Mickael Leclercq; Marion Narbebaru; Tabiwang N. Arrey; Nicolaie Bache; Clarisse Gotti; Claire Dauly; Dorte B. Bekker-Jensen; David Bouyssié; Maurice Boissinot; Michel G. Bergeron; Arnaud Droit; Proteomics platform and Computational Biology Laboratory - CHU Québec Université Laval Research Center, Québec, QC; Thermo Fisher Scientific, Bremen, Germany; Eevosep Biosystems, Odense, Denmark; Institut de Pharmacie et de Biologie Structurale, Université de Toulouse, CNRS, Toulouse, France; 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; William Russell; University of Texas Medical Branch at Galveston, Galveston, TX

WP 520 Quantitative Proteomics Reveals a Multifactorial Mechanism of Antifungal Drug Resistance; Margarita Semis; Daniel Roeth; Elizabeth Avery Henderson; Markus Kalkum; City of Hope, Duarte, CA

WP 521 HIV Phosphorylation Site Investigation Using MALDI-LTQ; Andre D. Dunkley; Kevin J. Mark; Pratikkumar Rathod; Emmanuel Chang; Department of Natural Sciences, LaGuardia Community College, Long Island City, NY; Department of Chemistry, York College, Jamaica, NY; 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; Meena Rajagopal; Adrian Zelazny; Aleksandra Nita-Lazar; NIH/NIAID, Bethesda, MD; NIH/CC/DLM, Bethesda, MD

PROTEOMICS: QUANTITATIVE II

WP 523 TMT-Integrator: An efficient analysis and multi-level report generation for labeling-based proteomics experiments; Hui-Yin Chang; Felipe Da Veiga Leprevost; Weiping Ma; Pei Wang; Bo Wen; Bing Zhang; Alexey I. Nesvizhskii; University of Michigan, Ann Arbor, MI; University of Michigan, Ann Arbor, MI; Icahn School of Medicine at Mount Sinai, New York, NY; Baylor College of Medicine, Houston, TX

WP 524 Temporal Mitochondrial Proteomic Analysis of Pancreatic β-Cells in Response to Lipotoxicity and Glucolipotoxicity; Min Li; Junjie Hou; Institute of Biophysics, CAS, Beijing, China

WP 525 Targeted Profiling of Epitranscriptomic Reader, Writer and Eraser Proteins in Radioresistant Breast Cancer Cells; Tianyu Qi; Weili Miao; Yinsheng Wang; 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; Shu-Yuan Cheng; Monika Dzierciatkowska; Elise Chameill; Weill Cornell Medicine, New York, NY; Department of Sciences, John Jay College of Criminal Justice, City University of New York, New York, NY; Biological Mass Spectrometry Core Facility, University of Colorado Denver, Aurora, Denver, Colorado

WP 527 Quantitative Proteomics Analysis of the Aminoglycoside Producer Streptomyces tenebrarius; Darwin Linard; Tingyu Pan; Yi Yu; Henry Lam; The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong; Wuhan University, Wuhan, China; The Hong Kong University of Science and Technology (HKUST), Clear Water Bay, Hong Kong
Investigation and Characterization of the Jumping Translocation Breakpoint (JTB) Protein using Mass Spectrometry based Proteomics; Madhuri Jayathirtha; Devika Channaveerappa; Kangning Li; Costel Darie; 
1Clarkson University, Potsdam, NY

Reducing compression effects and expanding the multiplex capabilities on a timsTOF Pro with PASEF; Michael Krawitzky; Christopher Adams; Matt Willetts; Tharan Srikumar; 1Bruker Daltonics, San Jose, CA; 2Bruker Daltonics, Billerica, MA

Proteomic Analysis of Large Cohorts with a Micro Pillar Array Capillary Column; Simion Kreimer; Qin Fu; Angela Mc Ardle; Kimia Sobhani; Cory Bystrom; Jennifer Van Eyk; 1Cedars-Sinai Medical Center, Los Angeles, CA

Quantitative Proteomics of Cytosolic Proteins Derived from Temozolomide-resistant Glioma; Milan Teraiva; Helene Perreault; Vincent Chen; 1University of Manitoba, Department of Chemistry, Winnipeg, Manitoba; 2Brandon University, Department of Chemistry, Brandon, Manitoba

Quantitative Proteomic and Phosphoproteomic Analysis of 36 Breast and Ovarian Cancer Cell Lines; Gary A. Bradshaw; Robyn Eisert; Caitlin E. Mills; Mailul Nariya; Marian Kalocsay; Peter K. Sorger; 1Harvard Medical School, Boston, MA

Comparative evaluation of different plasma preparation techniques by TIMS TOF Pro instrument for quantification of up to 1000 plasma proteins; Alexander Brzhovozkivsky; Alexey Kononikhin; Anna Bugrova; Maria Indeykina; Natalia Zakharova; Christoph H. Borchers; Eugene (evgeny) Nikolaev; Skolkovo Institute of Science and Technology, Moscow, Russia; 2Moscow Institute of Physics and Technology, Dolgoprudny, Russia; 3Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; 4McGill University, Montreal, QC; 5Institute of Energy Problems of Chemical Physics Russian Academy of Sci., Moscow, Russia

New Quadrupole-Ion Trap-Orbitrap Mass Spectrometer Combined with Real Time Search Enhances Proteome Coverage and Quantification Accuracy in Multiplexing Workflows; Xiangyun Yang; Xiujie Sun; Yue Zhou; 1Thermo Fisher Scientific, Shanghai, China

Establishing a Proteomics Pipeline for Developing Proto-Vertebrate Ciona intestinalis; Alexander Frese; Andrea Mariossi; Michael Levine; Martin Wühr; 1Princeton University, Princeton, NJ

Comparison of Protein Quantification in human plasma by TMT and DIA workflows; Renny Shang-Lun Lan; 2Aaron J. Storey; Austin L. Brown; Stefan H. Graw; Samuel G. Mackintosh; Stephanie D. Byrum; Ricky D. Edmondson; 1Arkansas Children’s Nutrition Center, Little Rock, AR; 2University of Arkansas for Medical Sciences, Little Rock, AR; 3Baylor College of Medicine, Houston, Texas

Laser Ablation Microsampling for Top-Down Mass Spectrometry; Remilekun O. Lawal; Fabrizio Donnarumma; Kermit Murray; 1Louisiana State University, Baton Rouge, LA

Towards an optimized protocol for denaturing top-down proteomics of complex proteomes; Zhichang Yang; Xiaojing Shen; Daoyang Chen; Liangliang Sun; 1Michigan State University, East Lansing, MI

Integration of 193 nm ultraviolet photodissociation and fragment ion protection to improve the sequence coverage of large proteins; Sean D Dunham; James D. Sanders; Jennifer S. Brodbelt; 1University of Texas at Austin, Austin, TX

Profiling of Lipid-transfer Proteins from Plasma Using Miniaturized AF4 Coupled with ESI-MS; Jin Yong Kim; Myeong Hee Moon; 1Yonsei University, Seoul, South Korea

Comprehensive characterization of antibody drug conjugates by CESI-MS; Andras Guttman; Bryan R Fonslow; Gabor Jarvas; 1Sciex, Brea, CA; 2University of Debrecen, Debrecen, Hungary; 3The Scripps Research Institute, La Jolla, CA

Adaptation of Native GELFrEE for HDL Particle Size Subtype Separation and Differential Apolipoprotein Proteoform Quantification; Cameron Lloyd-Jones; Henrique dos Santos Seckler; Allan Sniderman; Philip D Compton; John T. Wilkins; Neill L Kelleher; 1Northwestern University, Evanston, IL; 2Northwestern University, Evanston, IL/60208; 3McGill University, Montreal, QC; 4Northwestern University, Chicago, IL

Activated Ion Electron Transfer Dissection Enables Electron-Based Dissociation Following Proton Transfer Charge Reduction; Josh Hinkle; Christopher Mullen; Jean M Lodge; Romain Huguet; Michael S Westphall; Joshua J Coon; John E.P. Syka; 1ThermoFisher Scientific, San Jose, CA; 2University of Wisconsin-Madison, Madison, Wisconsin

MASH Explorer, A Universal and Comprehensive Software for Top-down Proteomics Empowered by Machine Learning Methods; Sean J. Mcilwain; Zhijie Wu; Kent Wenger; Molly Wetzel; Jake A. Melby;
Xiaowen Liu1, 7; Ruixiang Sun6; Irene M. Ong1, 5; Ying Ge3, 4, 5; 1Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI; 2Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; 3Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI; 4Human Proteomics Program, School of Medicine and Public Health, Madison, WI; 5Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 6Department of BioHealth Informatics, Indianapolis, IN - Indiana; 7Center for Computational Biology and Bioinformatics, Indiana University, Indianapolis, IN; 8Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; 9Department of Obstetrics and Gynecology, University of Wisconsin, Madison, WI

WP 546
Facilitating User Defined Proteomics Search Spaces with Customized UniProt XML Files; Joseph B Greer1; Ryan T Fellers1; Rich D Deduc1; Mick Greer2; David M Horn3; Kenneth R Durbin1; 1Proteinaceous, Evanston, IL; 2Thermo Fisher Scientific, Austin, TX; 3ThermoFisher Scientific, San Jose, CA

WP 547
Top-Down Proteomics of Myofilaments in Neonatal Swine Hearts throughout Development; Timothy Aballo1; Ziqing Lin1, 2; Elizabeth Bayne2; Trisha Tucholski3; Wuqiang Zhu4; Meng Zhao5; Ahmed Mahmoud6; Jianyi Zhang3; Ying Ge1, 2; 1Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 3Department of Biomedical Engineering, University of Alabama at Birmingham, Birmingham, AL

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) Zha1; Xiaoling Yuan1; Jinyuan Zhang1; Mike (qingtao) Huang2; Sudhakar Pai2; Luca Matassa1; Zhongping (john) Lin1; 1Frontage Laboratories Inc, Exton, PA; 2Akros Pharma Inc., Princeton, NJ

WP 549
Impact of Sampling Rate and Transition Summing on Assay Variability for Triple Quadrupole Based Quantitative Analysis; Wei Zeng1; Kevin P. Bateman1; 1Merck 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 lli1; Thomas Nolin1; 1University 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 Schauer1; Craig Sykes1; Amanda Poliseno3; Heather MA Prince1; Angela DM Kashuba1; 1University 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 Liu1; Mingming Wang1; Deping Cheng1; 1Alliance 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 Sahasrabuddhe1; Dylan Oakley1; Kui Chen1; John Mccarter1; 1Amgen Inc., Thousand Oaks, CA

WP 554
Determination of Nitrosamine impurities in Losartan Potassium drug substance using Triple Quadrupole Liquid Chromatography Mass Spectrometry; Chander Mani1; Saikat Banerjee1; 1Agilent Technologies, Haryana, India

WP 555
No Chiral Inversion for SEP-363856 in Humans by A Novel Chiral LC-MS/MS Analysis of Human Plasma from Clinical Trials; Yu-Luan Chen1; Yao Shi2; Amber Lafayette2; Kenneth S. Koblan1; Gerald Galluppi1; 1Sunovion Pharmaceuticals, Inc., Marlborough, Massachusetts; 2Labtech Diagnostics, Anderson, SC

WP 556
Simultaneous Determination of Risperidone, Olanzapine, Aripiprazole, Amisulpride, Quetiapine, Haloperidol, Zuclopenthixol, and Fluphenazine (8-in-1) in Human Plasma by LC-MS/MS; Yu-Luan Chen1; Junyi Yang2; Yu-Luan Chen2; John (zhongping) Lin2; 1Sunovion Pharmaceuticals, Inc., Marlborough, Massachusetts; 2Covance Laboratories, Madison, WI

WP 557
Method Validation for the Determination of Methadone in Human Serum by Liquid Chromatography Coupled to Mass Spectrometry (LC/MS/MS); Amber Awad1; Ana Celia Grenier1; Lawrence J. Andrade1; 1Dominion Diagnostics, North Kingstown, RI

WP 558
High-Sensitivity Measurement of Estrogens without Derivatization in Human Serum Using EVOLUTE® EXPRESS ABN Prior to LC/MS-MS Analysis; Mohamed Youssef1; M.rabie Al-Turkmani2; Petch Kaewsuya2; Suzanne Kamel-Mohamed2; Elena Gairloch1; 1Biotage, Charlotte, NC; 2Labtech Diagnostics, Anderson, SC

WP 559
5-plex Mass Defect-based Isobaric Multiplex Reagents for Carbonyl-Containing Compound (msSUGAR) Tags for Multiplex Quantification of N-glycans; Xiaorong Lin1, 2; Miyang Li3; Yuanjuan Lin1, 4; Lingjun Li1, 3; 1School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; 2College of Food Science, South China Agricultural University, Guangzhou, China; 3Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 4Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI; 5Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 6Department of BioHealth Informatics, Indianapolis, IN - Indiana; 7Center for Computational Biology and Bioinformatics, Indiana University, Indianapolis, IN; 8Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; 9Department of Obstetrics and Gynecology, University of Wisconsin, Madison, WI

WP 560
Short abstract, Poster PDF, and optional presentation video will be included.
**Analysis of Spatially Distinct Skin Sections by Laser Capture Microdissection and Microflow LC-MS/MS;**
Jason Barricklow; James Finley; Lindsay Tomlinson; Brett Hollingshead; Colleen Dosinha; Pfizer, Groton, CT

**Identification and Quantitation of Nitrosamine impurities in various pharmaceutical API and drug substances;** Sandeep Choudhary; Chandrasekar M; Aman Sharma; Manoj G Pillai; Sciex, Gurugram, India

**Quantitation of Multi Residues Antibiotics in Milk Using the SCIEX Triple Quad™ 3500 System;** Chandra Sekar; Sabari Nathan; Manoj G Pillai; Lakshmanan D; Jianru Stahl- Zeng; Sciex, Gurugram, India; Sciex Germany GmbH, Darmstadt, Germany

**LC/MS/MS Method development and validation of fosaprepitant (fAPT) and aprepitant (APT) in K3EDTA treated rat plasma;** Rachel Sun; Hasantha Jayaratna; Natasha Campbell; Scott Clark; Inotiv, West Lafayette, IN - Indiana

**Validated LC-MS/MS Assay for Quantitation of Venetoclax in Human K2EDTA Plasma;** Robert Clegg; Ashton Hjerstedt; Rachel Sun; Inotiv, West Lafayette, Indiana

**Method Development for the separation and determination of cis-/trans-ceftibuten in human plasma by LC-MS/MS;** Jingguo Hou; Xiaodong Zhu; Karin Keller; Shaolian Zhou; Worldwide Clinical Trials, Austin, TX

**ELECTROSPRAY IONIZATION VERSUS ATMOSPHERIC PRESSURE SPRAY IONIZATION FOR BIOANALYSIS OF ACETYLCOLINE FROM CEREBROSPINAL FLUIDS USING LIQUID CHROMATOGRAPHY–TANDEM MASS SPECTROMETRY;** Laszlo Prokai; Vien Nguyen; Daniel L. De La Cruz; Katalin Prokai-Tatrai; University of North Texas Health Science Center, Fort Worth, TX

**Rapid Quantitative Analysis of Fermentation Broth Samples to Assess Efficiency of Engineered Yeast Strain Turnover;** Rahul Baghla; Rolf Kern; Chang Liu; Axel Besa; Neil Walsh; SCIEX, Redwood Shores, CA; SCIEX, Concord, ontario; Sciex Germany GmbH, Darmstadt, Germany; Sciex, Warrington, United Kingdom

**Epigenetic Signatures that Regulate Caste Plasticity of Leafcutter Ants;** Michael Gilbert; Cristina M Brady; Benjamin A. Garcia; Shelley L Berger; University of Pennsylvania, Philadelphia, PA

**Multi-omics identifies the role of RNA splicing dysfunction in Alzheimer’s disease;** Xian Han; Ping-Chung Chen; Junmin Peng; St Jude Children’s research hospital, Memphis, TN; University of Tennessee Health Science Center, Memphis, TN 38163

**Analytical Deconvolution and Characterization of Mixed Phenotypic Subpopulations in Wild-Type Salmonella;** Michelle Reid; Alyson Hockenberry; Nicola Zamboni; Institute of Molecular Systems Biology, Department of Biology, ETH Zürich, Zürich, Switzerland; Institute of Biogeochemistry and Pollutant Dynamics, Department of Environmental Microbiology, ETH Zürich, Dübendorf, Switzerland

**Dynamic metabolic network modeling of a cytokine-induced mammalian cell cycle using time-course metabolomics and proteomics;** Ho-Joon Lee; Fangzhou Shen; Sriram Chandrasekaran; Yale University, New Haven, CT; University of Michigan, Ann Arbor, MI; University of Michigan, Ann Arbor

**R2-P2 rapid-robotic phosphoproteomics enables multidimensional cell signaling studies;** Mario Leutert; Ricardo Rodriguez-Mías; Noelle K Fukuda; Judit Villen; 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; \(^2\)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\(^5\); 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 Baltimore, Baltimore, MD; \(^2\)University of 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 deacetylase 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* 4; *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, 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* 2; *Romuald Huguet* 4; *Michael W. Bedford* 4; *Scott Peterman* 4; *John P Mcgeee* 1; *Philip D. Compton* 2; *Paul Thomas* 2; *Joshua Levitsky* 3; *Neil L Kelleher* 2;  
1*Northwestern University, Evanston, IL*; 2*Northwestern University, Evanston, IL*; 3*东北师范大学, 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 Budrero* 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*Biomognys AG, Schlieren, Switzerland*; 3*Lawrence Berkeley Laboratory, University of California, Berkeley, California*

**ThP 007**  
**Phosphoproteomics revealed activation of ATM signaling pathway in levalidomide resistant multiple myeloma:**  
*Santosh Renuse* 1, 2; *Yuan Xiao Zhu* 1; *Dong-Gi Mun* 1; *Anil K Madugundu* 1; *Kiran K Mangalaparthi* 1; *Chang-Xin Shi* 1; *A. Keith Stewart* 1, 2; *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; *Erdin Sertoglu* 1; *Harry V Vinters* 1; *Kym F Faull* 1; *Varghese John* 1; *Julian P Whitelegg* 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:**  
*Vanii V* 1; *Saikrishna S.B.* 1; *Rajesh Babu D.* 1; *Venkatesh S.* 1; *Vasan S.s.* 1; *Adiga S.K.* 1; *Varsha S.r.* 1; *Sachdeva G.* 1; *Seshagiri P.b.* 1;  
1*Indian Institute of Science, Department of Molecular Reproduction, Development and Genetics, Sir CV Ramam Road, Bangalore, India*; 2*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning, India*; 3*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning, Puttaparthi, India*; 4*Dept. of Biosciences, Sri Sathyasai Institute of Higher Learning, Puttaparthi, India*; 5*Manipal Ankur Andrology & Reproductive Services, Bangalore, India*; 6*Kasturba 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 Ramam 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, 2; *Alexandra C. Small* 3; *Mark Mclaughlin* 1; *Dorothy Mckeegan* 1; *Maureen Bain* 1; *Mangesh Bhide* 1; *Tom Preston* 1;  
1*University of Glasgow, Glasgow, UK*; 2*University of Glasgow, Glasgow, UK*; 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* 1; *Rebecca S Arnold* 1; *John A. Petros* 4, 5; *Facundo M. Fernandez* 1; *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 016  Proteograph, a novel multi-nanoparticle platform, enables rapid and deep proteomics profiling, significantly improving coverage, throughput, and scalability versus existing methods; John E. Blume1; Shadi Ferdosi1; Daniel Hornburg1; Matthew E. K. Chang3; Philip C. M. Ma1; Omid C. Farokhzad2; Mark R. Flory2; Patrick A. Everley3; 1Seer, Inc., Redwood City, CA; 2Cancer 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 Tumer1; Stephanie Frahs1; Xinzhu Pu1; Laura Bond1; Trevor Lujan1; Cindy Keller-Peck1; Julia Thom Oxford1; 1Boise State University, Boise, ID

ThP 014  Cathepsin B Dependent Cleavage Product of Serum Amyloid A1 Identifies Patients with Chemotherapy-Related Cardiotoxicity; Jia Fan1; Bo Ning1; 1Tulane University, New Orleans, LA

ThP 015  Metabolomics study reveal the protective effect of Apigenin on APAP-induced liver injury; Cheng Hu1; Yiqun Jia1; 1Shanghai University of Traditional Chinese Medicine, Shanghai, China

BIOMARKERS: QUANTITATIVE ANALYSIS III
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 Lacasse1,2; Vincent R. Richard1; Georgia Mitsa1; Oliver Poetz2; René Zahedi1; Alan Spatz1,5; Christoph H. Borchers1,4,8; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Department of Pathology, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 3Signatope GmbH, Reutlingen, Germany; 4Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 5Division of Pathology, Jewish General Hospital and McGill University Health Center, Montreal, QC; 6Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Engineering, Skolkovo Innovation Center, Moscow, Russia

ThP 017  High-throughput Proteomics Approach for Systematically Profiling Phosphotyrosine Signaling Complexes; Qian Kong1; 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 Kurono1; Satomi Niwayama2; 1FUJIFILM Wako Pure Chemical Industries, Ltd., Osaka, Japan; 2Muranor Institute of Technology, Muroran, Japan

ThP 019  Immunofluorescence LC/MS for the Quantitation of Mouse PD1, PD-L1 in Tumor for Drug/Target Characterization Study; Yoming Zhu1; Petia Shipkova1; Jacob Zalaznick1; Bogdan Slezcka1; Matthew Mazur1; Zheng Yang1; Karen Parrish1; Jesse Swanson1; Anwar Mutraza1; Timothy Ohl1; 1Bristol-Myers Squibb Company, Princeton, NJ

ThP 020  Rapid High-Throughput Profiling and Quantitation of Sialic Acids in Biotherapeutics; Anna Fong1; Ace G. Galermo1; John Yan1; Tom Rice1; Aled Jones1; Hamutal Bonen1; Gregory Staples1,2; Ted Haxo1; 1Agilent Technologies, Hayward, CA; 2Agilent Technologies, Santa Clara, CA

ThP 021  Novel target LC-MS methods to detect protein biomarkerin human serum extracellular vesicles; Fengping Li1; Lindsay King1; Hendrik Neubert1; 1Pfizer Inc., Andover, MA

ThP 022  Isolation and Determination of Cell Surface, Intracellular, ExtracellularPD-1 using Cell Surface Labeling; Huidong Gu1; Marissa Demichele1; Yue Zhao1; Brian Schmidt1; Yan J Zhang1; Renuka Pillutla1; Jianing Zeng1; 1Bristol-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 Zhang1; Mireille Tallandier2; Olivier Lacombe2; Eugeni Entchev2; James Beasley1; Ashlee R Stiles1; Sarah P Young1; 1Duke University Health System, Durham, NC; 2Inventiva 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 Hou1; Xiaolei Liu1; Tian-Sheng Lu1; Guangchun Zhou1; 1Medpace, Cincinnati, OH

ThP 025  Developing molecular-specific biomarker assays for IgA vasculitis with nephritis; Alyssa L. Hansen1; Ellenore P. Craine1; Audra A. Hargett1; Stacy D. Hall1; Bruce A. Julian1; Jan Novak1; Matthew B. Renfrow1; 1University of Alabama at Birmingham, Birmingham, AL

ThP 026  Quantification of creatinine in urine samples by High-Throughput Screening (HTS) using LDTD-MS/MS; Francis Briere1; Pier-Luc Plante1; Jean Lacoursière2; Serge Auger2; Jacques Corbeil1; Pierre Picard2; 1Université Laval, Québec, QC; 2Phytronix 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 Jiang1; Jihai Pang1; Nakia Spencer1; Quanyun Xu1; Anastasia Lopez1; Thomas Quill1; Jennifer Linares1; Angela Harris1; Jeffery Kovacs1; Timothy Heffernan1; Kang Le1; Michael Soth1; Phillip Jones1; 1MD 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; Captor Biosciences, Montreal, QC

ThP 029  LC-high resolution mass spectrometry for quantitative assay of advanced glycation end-products in plasma;  Hye Kyong Kweon1;  Edwin Miranda2;  Jacob M. Haus3;  1Department of Chemistry, University of Michigan, Ann Arbor, MI;  2School of Kinesiology, University of Michigan, Ann Arbor, MI;  3Department of Pediatrics, Shimane Medical School, Izumo, Japan;  4Shimadzu Corporation, Global Application Development Center, Columbia, Vancouver, BC;  5University of British Columbia, Vancouver, BC;  6Lifelabs Medical Laboratories, Burnaby, BC;  7Simon Fraser University, Burnaby, BC;  8University of Washington, Seattle, WA

ThP 030  A Microsampling Assay for the Quantitation of Vancomycin in Human Whole Blood;  Christina Vedara1;  Ganesh Moorthy1;  Kevin J Downes1;  Athena F Zuppa1;  1Children’s Hospital of Philadelphia, Philadelphia, PA

ThP 031  Determination of 25(OH)VD3 derivatives in LC-MS with special reversed-phase chromatographic columns;  Haijun An1;  Qiqi Tu1;  Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China

ThP 032  A Comparative proteomics study of mental disorders: Schizophrenia and Bipolar Disorder;  Ramesh Rajendran1;  Aparna Sundaresh2;  Vir Singh Negi2;  Vijayalakshmi M.a.1;  Kamalanathan A.s.1;  Centre for BioSeparation Technology, Vellore Institute of Technology, Vellore, India;  2Department 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. Borden1,2;  Armin Saatchi1;  Gregory W. Vandergrift1,2;  Nicole M. Esligar3;  Samuel Tobias3;  Mark Lyshysyn3;  Jan Palaitys3;  Erik T. Krog1,2;  Christopher G. Gill1,2,7,8;  Appl. Env. Res. Labs. (AERL), Vancouver Island University, Nanaimo, BC;  2University of Victoria, Victoria, British Columbia;  3BC Centre on Substance Use, Vancouver, BC;  4Vancouver Coastal Health Authority, Vancouver, BC;  5University of British Columbia, Vancouver, BC;  6Lifelabs Medical Laboratories, Burnaby, BC;  7Simon Fraser University, Burnaby, BC;  8University of Washington, Seattle, WA

ThP 034  Exemplary performance data for a Triple Quadrupole Mass Spectrometer in a simulated clinical LDT workflow;  Byungchul Ch1;  Mindy Gao1;  Kristine Van Natta1;  Terry Olney1;  Maurino Flora1;  John Glazier1;  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 Ma1;  Qianqian Li1;  Wenjing Liu1;  Zhengwei Jia1;  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 Trivedi1;  Shailesh Damale1;  Shaiendra anil Rane1;  Deepti Bhandarkar1;  Purushottam Sutar1;  Anant Lohar1;  Ashutosh Shelar1;  Navin Devadiga1;  Jitendra Kelkar1;  Pratap Rasam1;  Ajit Datar1;  Shimadzu Analytical (India) Pvt. Ltd, Mumbai, India

ThP 037  Control strategy for the matrix effect for actual study samples in regulated clinical analysis;  Jinhui Zhang1;  Arindam Dasgupta1;  Rubin Ayala1;  Jianghong Gu1;  Charles Bonapace1;  Sean Kassim1;  Patrick Faustino1;  FDA, Silver Spring, MD

ThP 038  Evaluation of a rapid LC-MS/MS method to measure simultaneously IDUA and IDS enzymes activities in dried blood spots;  Misa Tanaka1;  Tsusbasa Oguni1;  Yoshitomo Notsu1;  Tetsuo lida1;  Takanari Hattori1;  Jun Watanabe1;  Hironori Kobayashi1;  MS specialite, Yokohama, Japan;  2Clinical Laboratory Division, Shimane University Faculty of Medicine, Izumo, Japan;  3Shimadzu Corporation, Global Application Development Center, Kyoto, Japan;  4Shimadzu Corporation, MS Business Unit, Kyoto, Japan;  5Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan

ThP 039  Proteomic evaluation of ALA induced fluorescence in Glioblastoma to understand biological heterogeneity;  Saicharan Ghantasala1;  Deepatup Biswas1;  Aliasgar Moiyadi2;  Sridhar Epari3;  Sanjeeva Srivastava4;  Department of Biosciences and Bioengineering, IIT Bombay, Mumbai, India;  2Division of Neurosurgery, Department of Surgical Oncology, Tata Memorial Centre, Hombhah National University, Mumbai, India;  3Department of Surgical Pathology, Tata Memorial Centre, Hombhah National University, Mumbai, India;  4IIT Bombay, Mumbai, India

ThP 040  A rapid and highly sensitive LC-MS/MS method for bioanalysis of biotin in human plasma;  Peiling Hou1;  Dijohan Kesuma1;  Jie Xing1;  Shimadzu (Asia Pacific), Singapore, Singapore

ThP 041  Development and validation of a dried blood spot LC-MS/MS method for indomethacin analysis;  Whitney Nolte1;  Kim Gibson1;  Allison Scott1;  Tamorah Lewis1;  Children’s Mercy Hospital, Kansas City, Kansas City, MO

ThP 042  A High-Throughput Integrated HRAM-MS Method Enables IGF-1 Quantification, Targeted Variants Monitoring, and Untargeted Variants Screening in a Single Injection;  Yu Zhou1;  Xiaolei Xie1;  Kristine Van Natta1;  Bradley Hart1;  Shen Lu1;  Debadeep Bhattacharyya1;  Thermo Fisher Scientific, San Jose, California

ThP 043  Development and Implementation of an LC/MRM-MS Assay for a Panel of Antibiotics/Antifungals in Intensive Care Unit Clinical Settings;  Evgieniy V. Petroetchenko1;  Shaun Eintracht2;  Christoph H. Borchers1,3,4;
THURSDAY POSTERS (ThP) Pages 125-164 | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Department of Diagnostic Medicine, Jewish General Hospital, Montreal, Canada, Montreal, QC; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4Department 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 Kirkpatrick1; Christine L Skaggs2; Greta J Ren2; El Taher M Elgierari3; Lillian R Strumer4; Run Z Shi5; Nicholas E. Manicke6; 1Indiana University School of Medicine, Pediatric Infectious Disease, Indianapolis, IN; 2Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN; 3Stanford Health Care, Palo Alto, CA; 4Department of Pathology, Stanford University School of Medicine, Stanford, CA; 5Forensics 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 Kaur1; Dr. David Harman1; Dr. David A Mahns1; 1Western Sydney University, Campbelltown, Australia

ThP 048 Targeted serum glycoprotein profiling and quantification by LC-MS/MS for detection of ovarian cancer; Gege Xu1; Daniel Serie1; Ling Shen1; Padraig Buckley1; Maurice Wong1; Prasanna Ramachandran1; Rachel Rice1; Carlito Lebrilla1; Klaus Lindpaintner1; Hui Xu1; 1InterVenn Biosciences, South San Francisco, CA

ThP 051 High Resolution UHPLC-MS/MS Identification and Characterization of Superwarfarin Metabolites in Human Blood; Daniel Nosal1; Douglas L Feinstein2; Richard B. Van Bremesen1; 1Oregon State University - Linus Pauling Institute, Corvallis, OR; 2University of Illinois at Chicago - Department of Anesthesiology, Chicago, IL

CORPORATE POSTERS IV

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 Piperazine in a Tyrosine Kinase Inhibitor, Should We Throw the Red Flag? An In silico and Practical Bioactivation Approach.; Thamer Alsubi1; Adnan A Kadi1; Hany W Darwish1; 1King Saud University, Riyadh, Saudi Arabia

ThP 057 Workflow automation for lipidated peptide metabolite profiling; Tatiana Radchenko1; Jon Griffin2; Fabien Fontaine1; Ismael Zamora1, 3; 1Lead Molecular Design S.L., Sant Cugat de Valles, Spain; 2Zealand Pharma A/S, Copenhagen, Denmark; 3Molecular Discovery, Ltd., Borehamwood, United Kingdom

ThP 058 Biosynthesis and Structural Elucidation of Drug Metabolites by LC-MS and LC-SPE-NMR; Pingrong Liu1; Dongyue Xin1; Nina Gonnella1; Mitchell Taub1; Aaron Teitelbaum1; 1Boehringer 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 Sepehr1; Qiangen Wu1; Matthew S Bryant1; 1National 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 Chi1; Fumin Li1; Dennis Kraus1; Yonghua Ling1; Shane Roller2; 1PPD Inc, Madison, WI; 2Intarcia Therapeutics, Inc. Boston, MA, Boston, MA

ThP 061 Clinical analysis of creatinine reduction in bone marrow transplants induced by four immunosuppressants.; Wang Lei1; 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 Wang1; Kiran Chaudhari1; Yong Xu1; Ali Winters1; Xiaowei Dong1; Ran Liu1; Shaohua Yang1; 1University 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-Eng1; Ryan Lutz2; Bing Lu1; Kerry Fillgrove1; Melanie Anderson1; Dina Goykhman1; Eric Woolf1; 1Merck & 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 Zhang1; Jianbo Zhang2; Erhu Lu1; Zhongping (John) Lin1; John Haddock2; 1Frontage Laboratories, Inc., Exton, PA; 2Sarepta Therapeutics, Cambridge, MA
Application of Orbitrap ID-X Tribrid Mass Spectrometer for Metabolite Profiling; Ron Aoyama1; Kate Comstock2; Gilead Sciences Inc., Foster City, California; 2Thermo Fisher Scientific, San Jose, CA

NAFLD/NASH: Toward biologically-relevant and robust preclinical models for a successful selection of your drug clinical candidate; Rima Ait Beltacem1; Micheline Kergoat2; Alice Dufourn3; Fawzia Mouveau4; Sophie Raynaud; Laruanne Poncelet; Laurent Benelli; Fabien Pameld1; Sandrine Durand; Armel Nijman; Anthony Dessaux; David Bonnel; Valerie Autier; Jonathan Stauber; Imabiotech, Loos, France; 2Metabrain, Maisons-Alfort, France; 3Imabiotech, Billerica, Massachusetts

Quantitation of Contraceptive Hormones with Co-administered Antiretroviral Drugs in Human Plasma by LC-MS/MS; Jeffrey Jeppson1; Lee Winchester2; Kayla Campbell3; Timothy Mykris1; 1UNMC, Omaha, NE

Metabolomic analysis of effects of copper oxide nanoparticles and microparticles on microalgae Chlorella vulgaris; Lei Wang1; Xue Li Huang2; Anna Karen Carrasco Laserna3; Sam Li1; National University of Singapore, Singapore, Singapore

Strategies for homologous series detection — Investigating the fate of small water-soluble polymeric substances in a waste water treatment plant; Teresa Mairinger1; 2Martin Loos3; Juliane Hollender1, 4; 1EAWAG, Dübendorf, Switzerland; 2University of Natural Resources and Life Sciences-BOKU Vienna, Vienna, Austria; 3envi bee GmbH, Zurich, Switzerland; 4ETH Zurich, Zurich, Switzerland

Detection of volatile compounds emitted by bed bugs (Cimex lectularius L.) using selected-ion flow-tube mass spectrometry (SIFT-MS); Jesse L. Balcer1; Neil A. Spomer1; Aaron R. Ashbrook2; Mary E. Rushton3; Jeffrey R. Gilbert1; Ameya D. Gondhalekar2; Corteva Agriscience, Indianapolis, IN; Purdue University, West Lafayette, IN

Quantitative Determination of Per- and Polyfluoroalkyl Substances in Various Landfill Soils Using Ultra-High-Pressure Liquid Chromatography/Tandem Mass Spectrometry (UHPLC-MS/MS); Atiye Ahmadireskety1; Bianca F Da Silva2; Richard A. Yost1; John A. Bowden2; Chemistry Department, University of Florida, Gainesville, Florida; 2College of Veterinary Medicine, Department of Physiological Sciences, University of Florida, Gainesville, Florida

Analysis of PFAS compounds in Fish Tissue Using Offline Supercritical Fluid Extraction and LC-MS/MS; William Hedgepeth1; Yuka Fujito1; Ruth Marfil-Vega2; Logan Miller3; Shimadzu Scientific Instruments, Inc, Columbia, MD

Integrated metabolomics and lipidomics approach reveal dramatic polyunsaturated lysoglycerophospholipids accumulation in human lung fibroblasts exposed to fine particulate matter; Jong Cheol Shon1; Young Sang Kwon2; Hee-Jung Shim3; Min-Chul Shin1; Sung-Min Lee1; Jong-Hwan Kim2; Jong-Su Seo3; Korea Institute of Toxicology, Munsan-eup, Jinju, South Korea

Photolysis of Emerging Contaminants absorbed to Different plastics: Role of Surface Area; Xiolmara Martinez1; Daryl Giblin2; Nicolas Jozefowski1; Michael L. Gross2; M. Paul Chiarelli1; Loyola University, Chicago, IL; Washington University in St. Louis, St. Louis, Missouri

Metabolomics and lipidomics demonstrate two genetically similar lysogenic bacteria influence host metabolism based on growth substrate; Katarina A. Jones1; Jonelle T. R. Basso2; Kaylee R. Jacobs3; Courtney J. Christopher1; Haley B. Fielland1; Alison Buchanan1; Shawn R. Campagna1, 3; Department of Chemistry, University of Kansas, Knoxville, Tennessee; 2Department of Microbiology, University of Tennessee Knoxville, Knoxville, Tennessee; 3Biological and Small Molecule Mass Spectrometry Core, University of Tennessee Knoxville, Knoxville, Tennessee

Integrated Instrumental Approach for Characterization of Adsorbed Carcinogens and Heavy Metals on Firefighter Gear; Drew I Stolpman1; Allyson Cliet1; Shubhneet Warar1; Amaan Allan1; Debra Harris1; Touradj Solouki1; Baylor University, Waco, TX

Using machine-learning approaches and multivariate statistics to understand driving environmental forces in a large microbial marine metaproteome; Jaclyn Saunders1; Matthew McIlvin1; Dawn Moran1; Noelle Held1, 2; Chris Dupont1; Alyson E. Santoro1; Mak Saito1, 2; Woods Hole Oceanographic Institution, Woods Hole, MA; 2Massachusetts Institute of Technology, Cambridge, MA; 3J. Craig Venter Institute, Rockville, Maryland; 4University of California Santa Barbara, Santa Barbara, CA

Evaluating desalination wastewaters as a source of disinfection by-products in aquatic ecosystems; Danielle Westerman1; Leanne Powers2; Michael Gonsior3; Susan D. Richardson1; University of South Carolina, Columbia, SC; 2University of MaryLand Center for Environmental Science, Cambridge, MD

Biodegradation pathway of Anthraquinone dyes by a Novel Laccase from Trametes hirsute D7 fungus; Rafiqul Alam1; Fenny Clara Ardiati2; Nissa Nurfa Jrin2; Dede Heri Yuli Yanto2; Sunghwan Kim1, 3; Department of...
Environmental: Pharmaceuticals and Pesticides

**ThP 082**
Towards Single System for Total Water Analysis. LC-MS/MS screening of 325 PPCP Contaminants in Tap and Surface Water; Aurore Jaffuel¹; Mikael Levi¹; Jun Watanabe¹; 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 Itzel¹-²; Jill Kersten¹; Thorsten Teutenberg¹; Jan Stenzler³; Stephane Moreau⁴; Jochen Tuerk¹-²; Institut für Energie- und Umwelttechnik e.V. – IUTA (Institut of Energy and Environmental Technology), Duisburg, Germany; Centre for Water and Environmental Research (ZWU), University of Duisburg-Essen, Duisburg, Germany; Shimadzu Deutschland GmbH, Duisburg, Germany; 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 Christison¹; Jeffrey S Rohrer²; Thermo Fisher Scientific, Sunnyvale, CA; 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 Foss¹; Marjon Kuiper²; Boris Bartolec²; Peter Ringeling²; PerkinElmer, Shelton, CT; 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. Santos¹-²; Ana Luisa Mauviald³; Adrià Jaen-Gil¹-²; Antonio Marques³; Sara Rodríguez Mozaz³; Damia Barceló¹-², 4; Catalan Institute for Water Research (ICRA), Girona, Spain; University of Girona, Girona, Spain; Portuguese Institute for the Sea and Atmosphere (IPMA, I.P.), Lisbon, Portugal; IIDA-CECSIC, 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 Overfelt¹; Shahnaz Mukta¹; Alyssa Gasa¹; Christopher Mulligan¹; Illinois State University, Normal, IL

**ThP 088**
A Validated UHPLC-MS/MS Method for the Identification of Aliksiren Photodegradation Products in Water; Masho Hilawie Belay¹; Fabio Gosetti²; Emilio Marengo¹; Edoardo Pisano¹; Jessica Luisetti¹; Elisa Robotti¹; Department of Science and Technological Innovations, University of Piemonte Orientale, Viale T. Michel 11, 15121 Alessandria, Italy; Department of Earth and Environmental Sciences, University of Milano-Bicocca, Piazza della Scienza 1, 20126 Milano, Italy

**ThP 089**
Measurement of Underivatized Glyphosate and Other Polar Pesticides in Multiple Matrices Using Reversed-Phase Chromatography and Tandem Mass Spectrometry; Jean-Francois Roy¹; Jarod Grossman²; Agilent Technologies, Montreal, QC; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Wilmington, DE

**ThP 090**
Polar anticancer drugs in hospital and municipal wastewater by on-line extraction coupled to hydrophilic interaction liquid chromatography tandem mass spectrometry; Marc-Antoine Vaudreuil¹; Sung Vo Duy¹; Gabriel Munoz¹; Alexandre Furtos¹; Sébastien Sauvé¹; Université de Montréal, Montreal, QC

**ThP 091**
Determination of 33 pesticide residues in Lycium chinense Mill by GC-MS/MS; Xiaodan Yang¹; Chenyuan Zhang¹; Jian Kang¹; Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China

**ThP 092**
Analysis of Persistent Organic Pollutants in Drinking Water with Semi-Automated Solid Phase Extraction; Tom Hall¹; Ruud Addink¹; Fluid Management Systems, Watertown, MA

**ThP 093**
Removal of 14 HIV/AIDS related drugs and 15 frequently detected pharmaceuticals using Moringa protein/PVA nanofibers and Anaphile pandafibers; Tennesgen Girma Kebede¹; Simiso Dube-Nindi²; Mathew M Nindi³; UNIVERSITY OF SOUTH AFRICA(UNISA), Florida Park, Roodepoort, South Africa; UNISA, Florida Park, Roodepoort, South Africa

**ThP 094**
Elucidation of environmental fate of Maprotiline and Aliskiren drugs in natural waters: Identification of degradation products via HPLC-HRMS; Yuno P. F. Goncalves¹; Masho Hilawie Belay¹; Elisa Robotti¹; Claudio Medana¹; Alessandra Bianco Prevot¹; Paola Calza¹; University of Turin, Turin, Italy; University of Piemonte Orientale, Alessandria, Italy

**ThP 095**
Photodegradation of contaminants of emerging concern enhanced by dissolved organic matter derived from Pamvotis Lake sediments; Cristina Jimenez-Holgado¹; Sakkas Vasili¹; Richard Claire²; University of...
**FOOD SAFETY: GENERAL II**

**ThP 099**
Food monitoring feasibility study on cereal: non-targeted food contaminants detection method development and semi-quantification model application using LC/HRMS; Tingting Wang1; Jaanus Liigand2; Anneli Krueve2; Lene Duedahl-Olesen1; National Food Institute, Technical University of Denmark, Lyngby, Denmark; University of Tartu, Institute of Chemistry, Tartu, Estonia; 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 Chitranshi1; Jennifer C. Davis1; Evelyn H. Wang1; Christopher T. Gilles1; 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 Chakrabarty1; Wellin L Shelver1; David J Smith1; USDA, Fargo, ND

**ThP 102**
Development of simultaneous quantitative analysis of 18 anthelmintics in livestock products using liquid chromatography-tandem mass spectrometry; Hae-Ni Jung1; Seong-Kwan Kim1; Da-Hee Park1; Kyung-Hee Yoo1; Ho-Chul Shin1; konkuk university, Seoul, South Korea

**ThP 103**
Multiresidue Pesticides Analysis in Food Matrices Using an Enhanced Triple Quadrupole LC/MS System; Dan-Hui Dorothy Yang1; Kyle Covert1; Linfeng Wu1; Agilent Technologies, Santa Clara, CA

**ThP 104**
Direct Analysis of Glyphosate, Glufosinate and AMPA in Foods Using a Triple Quadrupole LC/MS/MS; Miho Kawashima1; Kota Ishioka1; Manami Kobayashi2; Junichi Hayakawa1; Shimadzu Corporation, Kyoto, Japan; Shimadzu Corporation, Hadano, Japan

**ThP 105**
Comprehensive quantitative and qualitative analysis of aflatoxins by UHPLC coupled to a quadrupole-Orbitrap MS; Laura E. Burns1; Dwayne E. Schnunk1; Viet Dang2; Dipankar Ghosh2; Iowa State Univ College of Veterinary Medicine, Ames, IA; Thermo Fisher Scientific, San Jose, CA

**ThP 106**
Veterinary Drugs Screening in Food Tissues Using LDTD-MS/MS Technology; Sylvain Letarte1; Pascal Belisle1; Serge Auger1; Jean Lacoursière1; Pierre Picard1; Phytronix Technologies, Quebec, QC

**ThP 108**
A multiresidue pesticide method using a modified quadrupole-Orbitrap MS for quantitation, screening and confirmation; Francesca Barbetti1; Charles T. Yang2; Debora D'adonna3; Christian Klass4; Dipankar Ghosh5; ISVIA S.r.L., Siena, Italy; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Milano, Italy; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

**ThP 109**
Are there PFAS in my water? A detailed look into bottled water; Brahm Prakash1; Eberhardt R Kuhn1; Ruth Marfil-Vega1; Shimadzu Scientific Instruments, Columbia, MD 21046

**ThP 110**
Separation of Mycotoxins by UHPLC-MS/MS using a Novel C18-based Stationary Phase; Geoff Faden1; MAC-MOD Analytical, Chadds Ford, PA

**ThP 111**
LC-MS/MS Analysis of Glyphosate, Glufosinate and AMPA in Foods with a Novel Ion Exchange/HILIC Column; Xiaoning Lu1; Dan Li1; Connor Flannery1; 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 Birukou1; Scott Young1; Gerson Graser1; Syngenta Crop Protection, LLC, Research Triangle Park, NC

**ThP 113**
Dispersive Liquid-Liquid Microextraction of Chloramphenicol and its Congener Species in Water, Meat and Milk -ESI-LCMS/MS; Ompelege E Kemokgatla1; Simiso Dube-Nindi1; Mathew M Nindi1; Residue Section, Botswana National Veterinary Laboratory, Gaborone, Botswana; UNIVERSITY OF SOUTH AFRICA(UNISA), Florida Park, Roodepoort, South Africa; UNISA, Florida Park, Roodepoort, South Africa

**ThP 114**
Determination of mixed contaminants (mycotoxins, pesticides & veterinary) in food by green microextraction-Orbitrap HRMS; Balete Esthethu Gbreyohannes1; Simiso Dube-Nindi1; Mathew M Nindi1;
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ThP 116
Heavy Metals in Pet Food: Changes in Heavy Metal Contamination in Pet Food over the past Decade; Patricia Atkins1; Tina Restivo2; Robert Lockerman2; 1SPEX CertiPrep, Metuchen, NJ; 2CEM 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; Prashanth Joseph1; Parul Thakur2; Saikat Banerjee1; Samir Vyas2; 1Agilent Technologies, BENGALURU, India; 2Agilent Technologies, Mumbai, India

FORENSICS II
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ThP 118
Investigation of fires by unconventional IID (Improvised Incendiary Device) and combustion residues on different materials by SPME-GC-MS; Marco Pazzi1; Sofia Ubaldi1; Eugenio Alladio1, 2; Fabrizio Malaspina2; Marco Vincenti1, 2; 1Dipartimento di Chimica, Universita’ degli Studi di Torino, Torino, Italy; 2Centro Regionale Antidoping e di Tossicologia “A. Bertinaria”, Regione Gonzole 10/1, 10043 Orbassano (Torino), Italy; 2Corpo Nazionale dei Vigili del Fuoco – Comando di Torino, Unità d’intervento Nucleare 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 Chambers1; Rabi A Musah1; 1University at Albany - SUNY, Albany, NY

ThP 120
Identification of the Environments of Equine Racing Facilities by LC-MS/MS; Rachel Proctor1; 2; Youwen You1, 2; Jaclyn R Missanello1, 2; Dominic M Giandonato1, 2; Joanne Haughan1; Mary A Robinson1, 2; 1University of Pennsylvania, Kennett Square, PA; 2PA 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 Romanova1, 2; Arash Etemadi1; 2; Reza Malekzadeh1; Jonathan D. Pollock1; 4; Jonathan V Sweedler1, 2; 1University of Illinois at Urbana-Champaign, Urbana, IL; 2Beckman Institute, UIUC, Urbana, IL; 3National Cancer Institute, Bethesda, MD; 4NIH, Bethesda, Maryland; 5Tehran University of Medical Sciences, Tehran, Iran; 6National 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 Gatmaitan1; Clara L Feider1; Diating Zhang1; Livia S Eberlin1; 1University 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 Mazzarino4; Fabio Comunità1; Xavier De La Torre1; Carlotta Stacchini1; Francesco Botrè1; 1Laboratorio 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 Yannell1; Manuel Gomez1; 1Agilent 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 Morato1; Patrick W. Fedick1, 2; Fan Pu1; R. Graham Cooks1; 1Purdue University, West Lafayette, IN; 2Research 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
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ThP 127
Unveiling the Hidden Complexity of Lithiated Hexose Dissociation Chemistry; Paul S. Soma1; Gary L. Glish1; 1University 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 Harts1; Yuko Lam2; Alina Theisen3; Christopher A. Wootton4; Tomes E. Morgan5; Mark P. Barrow1; Peter B. O’Connor1; 1University 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 Pandi1; Varatharajan Sabareesh1; 1Advanced 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 Cui1; Carolyn J. Cassady1; 1The University of Alabama, Tuscaloosa, AL
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**ThP 131**

Formation and fragmentation of lithium acetate cluster ions studied by ESI-Orbitrap MS & HCD MS/MS and molecular dynamics simulations; Bogdan Bogdanov; Jincheng Zhang; Andrew Parkins; Anil K Shukla; Michael McCallum; Shimadzu Scientific Instruments, Pleasanton, CA; Beijing Normal University, Beijing, China; Department of Chemistry, University of the Pacific, Stockton, CA; Retired, Richland, WA

**ThP 132**

Improved Electron Capture Dissociation Tandem Mass Spectrometry of Post-translationally Modified Peptides via Collision Induced Unfolding; Nhat Le; Ruwan T. Kurulugama; Varun V. Gakdi; Chae Kyung Jeon; Brandon Ruotolo; Kristina Hakansson; University of Michigan, Ann Arbor, Michigan; Agilent Technologies, Santa Clara, CA

**ThP 133**

Screening of a Basic Side Chain on Acetylated and Nonacetylated Peptoids; Yadwinder Singh Mann; Yuntao Zhang; Jianhua Ren; 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; Benjamin I Mckinnon; Nathan RB Boase; Berwyck LJ Poad; David L Marshall; Adam J Trevitt; Todd W Mitchell; Stephen J Blanksby; Queensland University of Technology, Brisbane, Australia; University of Wollongong, Wollongong, Australia; 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 Hu; Lei Li; Pengfei Guan; Pingping Wang; 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; Antony Membouef; CEMCA, Université de Brest, CNRS, Université Bretagne Loire, Brest, France

**ThP 137**

Fragmentation Behavior and Stability of Sulfated Peptides in Positive Ion Mode; Funju Jang; Y-Linh Tran; Kristina Hakansson; University of Michigan, Ann Arbor, Michigan

**ThP 138**

Dynamics of the Collision-Induced Dissociation Process in Quadrupole Ion Traps; Thomas Sebastian Neugebauer; Thomas Drewello; CEMCA, Université de Brest, CNRS, Université Bretagne Loire, Brest, France; Friedrich-Alexander-University Erlangen-Nuremberg (FAU), Erlangen, Germany

**FUNDAMENTALS: ION MOLECULE, ION/IION, ION/ELECTRON INTERACTIONS**

**ThP 139**

Formation of Carbon Dioxide Adducts from Carbamoxy Anions Generated During Gas-Phase Fragmentation of Anions Derived from Capsaicinoids; Annie Guan Wang; Zhaoyu Zheng; Athula B. Attygalle; Stevens Institute of Technology, Hoboken, NJ

**ThP 140**

High-Throughput Mass Spectrometry Platform for Gas-Phase Reaction Screening under Ambient Conditions; Dmytro S Kulyk; Abraham Badu-Tawiah; OSU, Columbus, OH

**ThP 141**

Vibrational excitation from electronic ground state to collisionally excited state enhances formation of w-ions from doubly charged peptides; Yury V. Vasil'ev; Michael C Hare; Joe Beckman; e-MSion, Inc., Corvallis, OR; Oregon State University, Corvallis, OR

**ThP 142**

Fragmentation and gas-phase reactions of diphenhydramine and analogues using AuNPs for Laser Desorption Ionization Mass Spectrometry; Claire Eberle; Katherine A. Stumpo; University of Scranton, Scranton, PA

**ThP 143**

Fragmentation and gas-phase reactions of diphenhydramine and analogues using AuNPs for Laser Desorption Ionization Mass Spectrometry; Claire Eberle; Katherine A. Stumpo; University of Scranton, Scranton, PA

**ThP 144**

Structural elucidation of sodium- and potassium-cationized phosphatidylcholines using electron induced dissociation; Tingting Yan; Matthias-Erich Born; Boone M. Prentice; 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; Emvia I. Calixte; Ana V. Quintero; Jacob B. Hatvany; Elyssia S. Gallagher; 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; Boone M. Prentice; 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; Stephan B.H. Bach; 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; Takashi Baba; 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; Oisin Shiels; Cameron Bright; Stephen J. Blanksby; Gabriel Da
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Silva; Adam Trevitt1; 1University of Wollongong, Wollongong, Australia; 2Queensland University of Technology, Brisbane, Australia; 3University of Melbourne, Parkville, Australia

ThP 150 Development of Negative Macromolecular Analyte Mass Analysis via Massive Ion Attachment (MAMIA): Anthony M. Pitts-McCoy1; Abdirahman M. Abdilllahi1; Kenneth W. Lee1; Scott A. Mcluckey1; 1Purdue University, West Lafayette, IN

ThP 151 Rate effects of submerged entrance barrier energetics on phenyl-type distonic radical ion reactions with acetylene; Paddy Kelly2; Oisín Shiels1; Cameron Bright1; Brett Burns1; Jack Turner1; Gabriel Da Silva2; Stephen J. Blanksby3; Adam Trevitt1; 1University of Wollongong, Wollongong, Australia; 2University of Melbourne, Parkville, Australia; 3Queensland University of Technology, Brisbane, Australia

FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS, CATALYSIS
ThP 152 Molecular mechanism of ISC iron–sulfur cluster biogenesis revealed by high-resolution native mass spectrometry; Cheng-Wei Lin1; Jacob W. McCabe1; David H. Russell1; David P. Barondeau1; 1Texas A&M University, College Station, TX

ThP 153 Simultaneous analysis of metal ions and organic components by HPLC-ESI-MS system; Kuck-Fai Li1; Pai-Chi Syue1; Ching-Yi Lien1; Kuo-Lung Ku1; 1National Chiayi University, Chiayi City, Taiwan

ThP 154 Real-time stepwise analysis of palladium catalysis; Gilian Thomas1; Scott McIndoe2; 1University of Victoria, Victoria, BC; 2University of Victoria, Victoria, British Columbia

ThP 155 Lithium Cation Basicity Estimates of Lignin β-0-4 Dimers; Kimberly R Dean1; Bert C. Lynn1; 1University of Kentucky, Lexington, KY

ThP 156 Hydrocarbon Formation Through Decomposition of Fatty Acids Catalyzed by Metal Complexes in the Gas Phase; Kevin E Parker1; Geethi Wergaoda1; Richard O’hair1; Victor Ryzhov1; 1Northern Illinois University, DeKalb, IL; 2CSIRO Manufacturing, Clayton, Australia; 3School 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 Corin1; María Elisa Crestoni1; Simonetta Fornarini1; Eslam Dabbish1; Emilia Sicilia1; Elisabetta Gabano1; Elena Perin1; Domenico Osella1; 1Università di Roma “La Sapienza”, Roma, Italy; 2Università della Calabria, Arcavacata di Rende, Italy; 3Università del Piemonte Orientale, Alessandria, Italy

FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS
ThP 158 Comparison of Fragmentation of Zn(II)-2Cys-2His Model Oligopeptide using Direct Dynamics Simulations and Mass Spectrometry; Abdul Malik1; William L. Hase2; Laurence A Angel1; 1Texas Tech University, Lubbock, TX; 2Texas Tech University - Lubbock, TX, Lubbock, TX; 3Texas 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 Valente1; Rabin Dhakal1; Kenji Yonemura1; 1The Ohio State University, Columbus, OH; 2University of Wollongong, Wollongong, Australia; 3University of Melbourne, Parkville, Australia

ThP 160 An Application of DFT for Characterizing the Energies of HDX for Solvated Glucose; Meg McCutcheon1; Emvia Calixte1; Emily Ziperman1; H. Jamie Kim1; Elyssia S. Gallagher1; 1Baylor University, Waco, TX

ThP 161 Comparing Collisional Cross Sections of N-Acetyl Modified Carbohydrates to Determine Computational Model Accuracy and Precision; Emily D Ziperman1; Emvia I Calixte1; Meg E McCutcheon1; Srinivas Pulipaka1; Elyssia S Gallagher1; 1Baylor University, Waco, TX

FUNDAMENTALS: NATIVE MS
ThP 162 Implementation of surface-induced dissociation on an Orbitrap EMR via the HCD cell using a reverse-entry ion source; Benjamin J Jones1, 2; Jacob W. McCabe3; Dalton T. Snyder1, 2; Zachary L VanAernum1, 2; Sophie R. Harvey1, 2; David H. Russell2, 3; Vicki H. Wysocki1, 2; 1The Ohio State University, Columbus, OH; 2Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; 3Texas 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 Wang1; Albert J. R. Heck1; Wenjun Tong1; Jianbin Wang1; 1Nanjing Normal University, Nanjing, China; 2Utrecht University, Utrecht, Netherlands; 4Tsinghua University, Beijing, China

ThP 164 Surface-induced dissociation of protein complexes on a cyclic ion mobility spectrometer; Dalton T Snyder1; Ben Jones1; Leon Lin1; Alyssa Stiving1; Sophie Harvey1; Vicki H Wysocki1; Darren Hewitt1; Jason Wildgoose2; Dale A. Cooper-Shepherd2; Jeffrey M. Brown2; Jakub Ujma2; Jim Lanridge2; 1The Ohio State University, Columbus, OH; 2Waters Technologies, Wilmslow, United Kingdom
Molecular weight determination of an adeno-associated virus based virus-like particle; Samuele Zoratto
Victor U. Weiss; Martina Marchetti-Deschmann; Elisabeth Mueller; Robert Pletzenauer; Juan Hernandez Bort; Guenter Allmaier; TU Wien, Vienna, Austria; Takeda Austria GmbH, Vienna, Austria

Native ESI MS for Deep Characterization of JMJD3 and JMJD3-Binder Interactions; Xidong Feng
Yue Feng; Timothy Foley; Dafydd Owen; Pfizer, Groton, CT; Spectrix Analytical Services, North Haven, CT; Pfizer, Cambridge, MA

Probing the gas-phase structure of lipoprotein nanodiscs using surface-induced dissociation; Sophie R Harvey
Zachary L Vanaernum; Marius M Kostelic; Michael T Marty; Vicki H Wysocki; The Ohio State University, Columbus, OH; University of Arizona, Tucson, AZ

A Microflow LC-MS Platform for Native Protein Analysis; Weimin Ni
Maoyin Li; Yan Han; Pan Mao; Daqing Wang; Newomics Inc., Berkeley, CA

Screening tagged proteins using online tandem affinity-buffer exchange chromatography with native mass spectrometry; Stella M. Lai
Zachary L. VanAernum; Florian Busch; Julia Baek; Terry Zhang; Kyle L. Fort; Rosa Viner; Vicki H. Wysocki; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Resource for Native Mass Spectrometry-Guided Structural Biology, The Ohio State University, Columbus, OH; Campus Mass Spectrometry Instrument Center, Mass Spectrometry and Proteomics, The Ohio State University, Columbus, OH; Thermo Fisher Scientific, Sunnyvale, CA; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Bremen, Germany

So HowBad is Ammonium Acetate for Native Mass Spectrometry? pH Changes During Nanoelectrospray Ionization (nESI) Quantified Using Fluorescence Imaging; Matthew F. Bush
Evan E Hubbard; Meagan Gadzuk-Shea; University of Washington, Seattle, WA; University of California, Riverside, Riverside, CA

Determination of 33 pesticide residues in Ginseng using gas chromatography-triple quadrupole mass spectrometry; Xiaoming Bao
Yan Gou; Jun Fan; Taohong Huang; Shimadzu (China) Co., Ltd, Chengdu, China; Sichuan Institute for Food and Drug Control, Chengdu, China; Shimadzu (China) Co., Ltd, Shanghai, China

Thermal Desorption-GCMS Method for Screening of Extractables in in Drug Packaging Materials; Cynthia Melanie Lahey
Elgin Guo Wei Ting; Dheeraj Handique; Yukihiro Kudo; Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; Shimadzu Analytical (India) Pvt Ltd, Mumbai, India; Shimadzu Corporation, Kyoto, Japan

Thermal Desorption-GCMS Method for Screening of Extractables in in Drug Packaging Materials; Cynthia Melanie Lahey
Elgin Guo Wei Ting; Dheeraj Handique; Yukihiro Kudo; Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; Shimadzu Analytical (India) Pvt Ltd, Mumbai, India; Shimadzu Corporation, Kyoto, Japan

VOC Capturing Method for Odor Smell Analysis by GC-MS; Takeshi Furushashi
Shigenori Ota; Anicom Specialty Medicinal Institute, Yokohama, Japan; GL Sciences Inc., Shinjuku-Ku, Japan

Medical Diagnostics by GC-MS with Cold EI – Lipids and Drugs Analysis in Raw Blood; Benjamin Neumark
Aviv Amirav; Tel Aviv University, Tel Aviv, Israel; Aviv Analytical, Hod Hasharon, Israel

Integrated qualitative analysis of polymer samples by a pyrolysis - gas chromatography combined with high-resolution mass spectrometry; Masaaki Uebukata; Ayumi Kubo; Kenji Nagatomo; Robert A. Diaspaule; JEOL, Ltd., Tokyo, Japan; JEOL USA, Inc., Peabody, MA

Optimum molecular descriptors based on 89 machine learning methods for predicting the recovery rate of pesticides in crops by GC-MS; Takeshi Serino
Yoshizumi Takigawa; Sadao Nakamura; Tarun Anumol; Md. Altaf-Ul-Amin; Shigehiko Kanaya; Agilent Technologies, Hachioji, Japan; Nara Institute of Science and Technology, Ikoma, Japan; Agilent Technologies, Wilmington, DE

IDENTIFYING BEST APPROACHES TO ANALYZE VOLATILE EXTRACTABLES FROM MEDICAL DEVICES; Samantha l Wickramasekara
Keaton Nahan; Eric Sussman; Berk Oktem; US.Food and Drug Administration, Silver Spring, MD

Determination of Dioxin in Food by GC/MSMS coupled with Boosted Efficiency Ion Source (BEIS); Ge Yin
Feifei Tian; Jun Fan; Masato Takakura; Koki Tanaka; Eberhardt Kuhn; Daojing Wang; Feng; Timothy Foley; Dafydd Owen; Pfizer, Groton, CT; Spectrix Analytical Services, North Haven, CT; Pfizer, Cambridge, MA

Quantitative Multiplexed Elemental (C, H, N and S) Detection in Complex Mixtures using Gas Chromatography-combustion-mass spectrometry; Laura Freije-Carrelo; Javier Garcia-Bellido; Laura Alonso Sobrado; Mariella Moldovan; Marco Piparo; Brice Bouyssiere; Pierre Giusti; Jorge Ruiz-Encinar; Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, Spain; TOTAL, Harfleur, France; International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, Harfleur, France; Universite de Pau et des Pays de l’Adour, E2S UPPA, CNRS, IPREM, UMR5254, Pau, France
H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION

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ThP 193  Perfluoroalkyl Substances (PFAS) Bind to Human Plasma Transthyretin (hTTR) in the Thyroxine-Binding Site: an HDX-MS Study; Danielie Peterle1; Laura Aequassali1; Luca De Toni2; Carlo Foresta2; Barbara Spolaore2; Vincenzo De Filippis1; 'Department of Pharmaceutical and Pharmacological Sciences, Laboratory of Protein Chemistry and Molecular Haematology, University of Padua, Padua, Italy; 2Department 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 Lambert1; Jennifer Ross1; Cecilia Piergentili2; Kevin Waldron3; Didi He3; Jon Marles-Wright4; Colin Logan Mackay1; David Clarke5; 'University of Edinburgh, Edinburgh, United Kingdom; 2University of Newcastle, Newcastle, United Kingdom; 3University 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 Mattice1; Angela Patterson2; Bennett Streit3; John Peters2; Jennifer Dubois1; Brian Booth1; 'Montana State University, Bozeman, MT; 2Washington State University, Pullman, WA

ThP 196  Thermal activation networks in adenosine deaminase identified using hydrogen/deuterium exchange mass spectrometry; Anthony T. laverone1; Shuaihua Gao1; Samuel L. Barrow1; Emily J. Thompson1; Wenju Zhang2; Judith P. Klinman1; 1University of California, Berkeley, Berkeley, CA; 2University 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 Tremblay1; Richard W Vachet1; Eric Graban2; John E. Hale3; Robert C. Vaughn2, 3; 1University of Massachusetts Amherst, Amherst, MA; 2QuarryBio LLC, Bloomington, IL; 3Indiana University, Bloomington, IN

ThP 199 Two Binding Modes, One Nuclear Receptor: Analyzing Chemopreventative Rexinoids using Hydrogen Deuterium Exchange Mass Spectrometry; Nathalia Melo1; Zhengrong Yang1; Sejong Bae1; Venkatram Atigadda1; Donald D. Muccio1; Matthew Renfrow1; 1University of Alabama at Birmingham, Birmingham, AL

ThP 200 Conformational Dynamics of TMD-type Extended Spectrum β-Lactamases as Revealed by HDX-MS; Tez Fung Wong1; Pui Kin So1; Zhongping Yao1; 1The 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 Gramlich1; Henry C.W. Hays2; Dieter Stoll1, 3; Sandra Maier1; Anne Zeck1; 1Natural and Medical Science Institute at the University of Tuebingen, Tuebingen, Germany; 2MedAnnex, Edinburgh, United Kingdom; 3University 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 Lermyte1, 2; Emeline Hanozin3; Thomas Timlan4; Johann Far2; Loic Quintron2; Edwin De Pauw2; Gauthier Eppe5; 1University of Warwick, Coventry, University Kingdom; 2University of Liege, Liege, Belgium

ThP 204 Characterizing Small Molecule Inhibitors of CK2 Kinase Subunit a by HDX-MS; Darby J Ball1; Paul Brear2; Marko Hyvönen3; Sheena D’arcy4; 1University of Texas at Dallas, Richardson, TX; 2Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom; 3Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom; 4Department 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 Karageorgos1, 2; Sergiy Tuykhenko2; Girija Rajarshi3; Kyle Anderson3; Jeffrey W Hudgens1; Mahmoud Nasr3; Nikolai Zvonok2; Jason Guo4; Kiran Vemuri2; Gerhard Wagner2; Alexandros Makriyannis2; 1NIIST, Rockville, MD; 2Northeastern University, Boston, MA; 3Harvard 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 Kihn1; Patrick L. Wintrobe1; Daniel J. Deredge1; 1University of Maryland School of Pharmacy, Baltimore, MD

ThP 207 Refined Analysis of Calprotectin-Calculo Binding by Use of Three Titration MS Measurement Methods: HDEX, Sharp-break HDEX and Native Spray; Jagat Adhikari1; Jules R. Stephan2; Don L Rempel1; Elizabeth M. Nolan2; Michael L. Gross1; 1Department of Chemistry, Washington University at St Louis, St. Louis, MO 63103; 2Department 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 BAG-1L, using HDX-MS; Ezgi Basturk1; Ozge Tatli1, 2; Gizem Dinler Doganay1; 1Istanbul Technical University, Istanbul, Turkey; 2Istanbul 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. Jethva1; Alex W. Wessel2; Christopher A. Nelson3; Nurgun Kose4, 5, 6; James E. Crowe, Jr.4, 5, 6; Michael S. Diamond2, 3, 7, 8; Daved H. Fremont3, 7, 8; Michael L. Gross1; 1Department of Chemistry, Washington University in St Louis, Saint Louis, MO-63110; 2Department of Medicine, Washington University School of Medicine, Saint Louis, MO-63110; 3Department of Pathology and Immunology, Washington University School of Medicine, Saint Louis, MO-63110; 4Vanderbilt Vaccine Center, Vanderbilt University Medical Center, Nashville, TN-37232; 5Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN-37232; 6Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN-37232; 7Department of Molecular Microbiology, Washington University School of Medicine, Saint Louis, MO-63110; 8Department 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 Srinivasu1; Athina G Portaliou1; Anastassios Economou1; Spyridoula Karamanou1; 1KU Leuven, Leuven, Belgium

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**HIGH MASS ACCURACY/HIGH PERFORMANCE MS: APPLICATIONS AND INSTRUMENTATION**

**ThP 211** Towards Applying High Resolution Mass Spectrometry for Quantitative Source Apportionment: Evaluating Matrix Effects and Non-target Signature Fidelity; Katherine T Peter1; Zhenyu Tian2; Christopher Wu3; Edward P Kolodziej4, 5; John Kucklick1; 1National Institute of Standards and Technology, Charleston, SC; 2Center for Urban Waters, University of Washington Tacoma, Tacoma, WA; 3University of Washington, Seattle, WA

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**Imaging MS:** Method Development

**ThP 220**

**A high efficient and wide coverage mass spectrometry imaging method for broad functional metabolite discovery in ischemic stroke model:** Zixuan Wang; Ran Yang; Xin Li; Zeper Abliz 1, 2; 1Institute of Materia, Chinese Academy of Medical Science and Peking Union Medical College, Beijing, China; 2Minzu 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 2; Faye Cruickshank 3; C. Logan Mackay 4; Ron M.A Heeren 5; Diego F Cobice 1; 1Mass Spectrometry Centre, Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University, Coleraine, United Kingdom; 2Dutch Screening Group, Maastricht, Netherlands; 3The Nutrition Innovation Centre for Food and Health (NICHE), Biomedical Sciences Research Institute (BMSRI), School of Biomedical Sciences, Ulster University, Coleraine, United Kingdom; 4Scottish Instrumentation and Research Centre for Advanced Mass Spectrometry (SIRCAMS), EaSTCHEM School of Chemistry, University of Edinburgh, Edinburgh, United Kingdom; 5M4I 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 1, 3; Klaus Dreisewerd 1, 3; 1Institute of Hygiene, University of Muenster, Muenster, Germany; 2Center for Proteomics and Metabolomics, Leiden, Netherlands; 3Interdisciplinary 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; 1Johns 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 1; Chelsea Nikula 2; Alex Dexter 2; Adam Taylor 2; Richard Goodwin 3; Zoltan Takats 1; Josephine Bunch 1, 2; 1Imperial College London, London, United Kingdom; 2National Physical Laboratory, Teddington, United Kingdom; 3AstraZeneca, 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 1; Catherine Rawlins 1; Simona Salivo 1; Shimadzu Corporation, Kyoto, Japan; Shimadzu Corporation, Kyoto, Japan; 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 Flint1; Gregory Hamm2; Neil A Cross1; Laura M Cole1; David P Smith1; Richard Goodwin2; Malcolm R Clench1; 1Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom; 2Pathology, 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 Muller1; Ann M. Farese2; Thomas J. MacVittie2; Maureen A. Kane1; 1University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; 2University of Maryland, School of Medicine, Department of Radiation Oncology, Baltimore, MD

ThP 228  Method Development for using AuNPs in Mass Spectrometry Imaging; Tyler M. Bielinski1; Nolan K Mclaughlin1; Caitlin M. Tressler1; Eric Barton2; Kristine Glunde2; Katherine A. Stumpo3; 1University of Scranton, Scranton, PA; 2Johns Hopkins University School of Medicine, Baltimore, MD

ThP 229  Imaging Mass Spectrometry of Insoluble Proteins; Kevin L. Schey1; David M Anderson2; Zhen Wang1; 1Vanderbilt University, Nashville, TN; 2Vanderbilt University, Nashville, TN

ThP 230  MALDI mass spectrometry imaging in aqueous model systems; Elisabeth Schirmer1, 2; Axel Treu1; Sven Ritschar3; Stefan Schuster3; Christian Laforsch4; Andreas Römpp1; 1Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; 2Chair of Animal Physiology, University of Bayreuth, Bayreuth, Germany; 3Chair 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-Credo1; Tejaswi Kalavacherla1; Erin M. Schuman2; Hartmut Michel1; Julian D. Langer1, 2; 1Max Planck Institute of Biophysics, Frankfurt, Germany; 2Max 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 Mattson1; Akos Vertes1; 1The 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 Samenuk1; Stephan B.H. Bach2; Adalberto Pérez De León3; 1University of Texas at San Antonio, San Antonio, TX; 2University of Texas in San Antonio, San Antonio, TX; 3Knipling-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 Ikegawa1; Yumiko Toyama2; Yume Mukasa2; Inori Shintani2; Takayuki Ohmura3; Masahiro Kotani3; Akira Tashiro3; Hartmut Michel1; Julian D. Langer1, 2; 1Max Planck Institute of Biophysics, Frankfurt, Germany; 2Max Planck Institute for Brain Research, Frankfurt, Germany

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 Granborg1; Svend Kaasgaard2; Christian Janfelt3; 1University of Copenhagen, Novozymes A/S, Kongens Lyngby, Denmark; 2Novedigm A/S, Kongens Lyngby, Denmark; 3University 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 Chen1, 2; Jun Han1, 3; Juncong Yang1; Zhenzhong Zhang1; Christoph H. Borchers1, 4, 5, 6, 7; 1University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC; 2School of Pharmaceutical Sciences, Zhengzhou University, Zhengzhou, China; 3Division of Medical Sciences, University of Victoria, Victoria, BC; 4Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 5Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 6Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia; 7Department 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 Zhang1; Xudong Shi2; Nhu Vu1; Yatao Shi1; Miyang Li3; Bin Wang1; Lingjun Li1, 3; 1School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; 2Department of Surgery, University of Wisconsin-Madison, Madison, WI; 3Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222
ThP 240  Development of high sensitivity mass spectrometry imaging based on DIUTHAME chip; Masahiro Kotani1; Takayuki Ohmura1; Akira Tashiro1; Yasuhide Naito1; 1HAMAMATSU PHOTONICS K.K., Iwata City, Shizuoka Pref., Japan; 2The Graduate School for the Creation of New Photons Industries, Hamamatsu, Japan

ThP 241  Combining crown ether host-guest chemistry with mass spectrometry imaging to reveal dynamic sodium and potassium levels in tissue; Leonidas Matvyrodakis1; Kyle Daniel Duncan1; Ingela Lanekoff1; 1Department 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; Shin Muramoto; National Institute of Standards and Technology, Gaithersburg, MD

ThP 243  Lipid Analysis using Select Matrices with MALDI-2 Post-ionization for Advanced Imaging Applications; Josiah C Mcmillen1, 2; Jarod A. Fincher2, 3; Jeffrey M Spraggins1, 2, 3; Richard M Caprioli1, 2, 3, 4, 5; 1Department of Chemistry, Vanderbilt University, Nashville, TN; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Pharmacology, Vanderbilt University, Nashville, TN; 5Department of Medicine, Vanderbilt University, Nashville, TN

ThP 244  Comparative Analysis and Peptide Mapping of Ethanol and Formalin-Fixed Alzheimer's Human Brain Tissue; Savannah Dyer1; Andrea R Kelley1; Xiongwei Zhu2; George Perry1; Stephan B.H. Bach1; 1The University of Texas at San Antonio, San Antonio, TX; 2Case Western Reserve University, Cleveland, OH

ThP 245  On tissue-derivatization of lipopolysaccharide for detection of lipid A using MALDI MSI; Hwoi Ky Yang1; Courtney E Chandler1; Francesca M Gardner1; David Varisco1; David R Goodlett1, 2; Robert K Ernst1; Alison J. Scott1, 3; 1University of Maryland School of Dentistry, Baltimore, Maryland, MD; 2University of Gdansk, International Center for Cancer Vaccine Science, Gdansk, Poland; 3Maastricht 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; Katerina V Djambazova1, 2; Lukasz Miga3; Dustin Klein2; 4; Emilio S Rivera2; 4; Elizabeth Kathleen Neumann2; 1Vanderbilt University Department of Chemistry, Nashville, TN; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 3Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; 4Vanderbilt University, Department of Biochemistry, Nashville, TN; 5Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 6Mass Spectrometry Research Center, Nashville, TN; 7Department of Medicine, Vanderbilt University, Nashville, TN; 8Department 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; Vanna Dent1; Isabella Piga1; Sonia Guarnieri1; Francesca Clerici1; Clizia Chinello1; Giuseppe Paglia1; Fulvio Magni2; Andrew Smith1; 1Clinical Proteomics and Metabolomics Unit, Department of Medicine and Surgery, University of Milano-Bicocca, Vedano al Lambro, Italy; 2Biomolecular Sciences Research Centre, Sheffield-Hallam University, Sheffield, United Kingdom

ThP 248  Mapping Spatial Distributions of Drug Candidates for Inflammatory Bowel Disease with MALDI Mass Spectrometry Imaging; Meng Xu1; Dylan Nicholas Tabang1; Bing Tian1; Allan R Brasier1; Jia Zhou1; Lingjun Li1, 4; 1Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53705-2222; 2University of Texas Medical Branch at Galveston, Galveston, TX; 3University of Wisconsin-Madison, Madison, Wisconsin; 4School 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; Mary King1; Robert Yuan2; Jeremy Chen2; Isabel Sario1; Shirley Li1; Oscar Ekpenyong2; Janica Wong2; Jennifer Yearley2; Luis Zúñiga2; Maribel Beaumont2; Jin-Hwan Han2; Livia S Eberlin1; 1University of Texas at Austin, Austin, TX; 2Merck & Co., Kenilworth, NJ

ThP 250  Cutaneous drug delivery of tofacitinib in vehicles containing dexamethasone or sodium lauryl sulphate; Anne Mette Handler1, 2; Mariam Fallah1, 2; Gitte Pommeggaard Pedersen2; Kim Troensegaard Nielsen2; Christian Janfelt1; 1University of Copenhagen, Copenhagen, Denmark; 2LEO Pharma A/S, Ballerup, Denmark

ThP 251  Spatial metabolomics to trace metabolic deregulation and pathological heterogeneity in MYC-driven mammary gland tumours; Adam J Taylor1; Avinash Ghanate2; Peter Kreuzaler2; Yulia Panina2; Spencer A Thomas1; Alex Dexter1; Alejandro Suarez-Bonett3; Simon L Priestnall1; Ian S Gilmore1; Greg Mcmahon1; Zoltan Takats2; Maria Yuneva2; Josephine Bunch1, 2; 1National Physical Laboratory, Teddington, United Kingdom; 2The Francis Crick Institute, London, United Kingdom; 3The Royal Veterinary College, North Mymms, United Kingdom; 4Imperial College London, London, United Kingdom
Identification of phospholipid abundances in tissues of marine bivalves; Patric Bourceuau\textsuperscript{1}; Benedikt Geier\textsuperscript{1}; Dolma Michellod\textsuperscript{2}; Manuel Liebeke\textsuperscript{1}; \textsuperscript{1}Max Planck Institute for Marine Microbiology, Bremen, Germany

Low abundant metabolites/oxidized lipids imaging in single cells undergoing ferroptosis using H\textsubscript{2}O\textsubscript{2} gas cluster ion beam secondary ion mass spectrometry (H--2O-GCIB-SIMS); Hua Tian\textsuperscript{1}, \textsuperscript{2}; Louis J. Sparvero\textsuperscript{3, 4}; Andrew A. Amoscato\textsuperscript{3, 4}; Valerian E. Kagan\textsuperscript{3, 4, 5}; Hüllya Bayır\textsuperscript{3, 4, 5}; Nicholas Winograd\textsuperscript{3}; \textsuperscript{1}Department of Chemistry, Pennsylvania State University, University Park, PA; \textsuperscript{2}Materials Research Institute, Pennsylvania State University, University Park, PA; \textsuperscript{3}Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; \textsuperscript{4}Center for Free Radical and Antioxidant Health, University of Pittsburgh, Pittsburgh, PA; \textsuperscript{5}Department of Critical Care Medicine, and Safar Center for Resuscitation Research, University of Pittsburgh, Pittsburgh, PA

Modification of lipid expression in AKI kidney and possible reversion with Ferrostatin treatment studied by MALDI-IMS; Lucia Martin-Sanz\textsuperscript{1}; Olatz Fresnedo\textsuperscript{2}; Ana Belen Sanz Bartolomé\textsuperscript{3}; Jose A Fernández\textsuperscript{3}; Alberto Ortiz Arduan\textsuperscript{3}; \textsuperscript{1}Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; \textsuperscript{2}School of Pharmacy, University of Wisconsin-Madison, Madison, WI; \textsuperscript{3}Davies Heart and Lung Research Institute, The Ohio State University, Columbus, Ohio; \textsuperscript{4}Department of Surgery, University of Wisconsin-Madison, Madison, WI; \textsuperscript{5}Department of Chemistry, University of Wisconsin-Madison, Madison, WI

Spatiotemporal Dynamics of Bioactive Lipids in Arteries Undergoing Restenosis Observed and Identified at High Spatial Resolving Power; Gregory L Fisher\textsuperscript{1}; Yatao Shi\textsuperscript{2}; Jillian Johnson\textsuperscript{2}; Bowen Wang\textsuperscript{2}; Bingming Chen\textsuperscript{2}; Go Urabe\textsuperscript{2}; Xudong Shi\textsuperscript{3}; K. Craig Kent\textsuperscript{2}; Lian-Wang Guo\textsuperscript{2}; Lingqiu Li\textsuperscript{2, 5}; \textsuperscript{1}Physical Electronics, Chanhassen, MN; \textsuperscript{2}School of Pharmacy, University of Wisconsin-Madison, Madison, WI; \textsuperscript{3}Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN; \textsuperscript{4}Department of Physiology, Fac. of Medicine and Nursing, University of the Basque Country(UPV/EHU), Leioa, Spain; \textsuperscript{5}Laboratory of Nephrology, IIS-Foundation Jimenez Diaz, Madrid, Spain

DESI-MS imaging to visualize the spatial distribution of xenobiotics and endogenous lipids in the skin; Wei Rao\textsuperscript{1}; Susan Slade\textsuperscript{2}; Emmanuelme Claude\textsuperscript{1}; Emrys Jones\textsuperscript{1}; Frédéric Mété\textsuperscript{1}; Julie Quartier\textsuperscript{2}; Maria Lapteva\textsuperscript{2}; Yogeshwar Kalia\textsuperscript{2}; \textsuperscript{1}Waters Corporation, Wilmslow, United Kingdom; \textsuperscript{2}University of Geneva, Geneva, Switzerland

Diagnosing breast cancer in FFPE tissue samples using DESI-MSI; Olof Gerdur Isberg\textsuperscript{1, 2}; Paolo Inglese\textsuperscript{2}; Dipa Gurung\textsuperscript{2}; Hiromi Kudo\textsuperscript{2}; Sigridur Klara Bodvarsdottir\textsuperscript{1}; Jon Gunnlaugur Jonasson\textsuperscript{2}; Margret Thorsteinsdottir\textsuperscript{1}; Zoltan Takats\textsuperscript{3}; \textsuperscript{1}University of Iceland, Reykjavik, Iceland; \textsuperscript{2}Imperial College London, London, United Kingdom; \textsuperscript{3}Landspitali -The National University Hospital of Iceland, Reykjavik, Iceland

Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS) subcellular imaging of low abundance phosphatidylethanolamine metabolites in traumatized brain neurons; Li, J. Sparvero\textsuperscript{1}; Hua Tian\textsuperscript{2}; Wanyang Sun\textsuperscript{1}; Andrew A. Amoscato\textsuperscript{1}; Simon C. Watkins\textsuperscript{1}; Nicholas Winograd\textsuperscript{2}; Valerian E. Kagan\textsuperscript{2}; Hüllya Bayır\textsuperscript{1}; \textsuperscript{1}University of Pittsburgh, Pittsburgh, PA; \textsuperscript{2}The Pennsylvania State University, University Park, PA

MALDI-Imaging Mass Spectrometry of Virgin and Bleached Human Hair: An Analytical Technique to Identify "Moisturized" Hair Biomarkers; Stella K Betancourt\textsuperscript{1}; Yi Fan\textsuperscript{1}; Wendy Kin Man Chan\textsuperscript{1}; Shouxun Zhao\textsuperscript{1}; \textsuperscript{1}BASF, Tarrytown, NY

Multi-Modal Mass Spectrometry Imaging of an Animal Model of High-Grade Serous Ovarian Cancer Provides Deeper Coverage; Clint M. Alfaro\textsuperscript{1}; Olga Kim\textsuperscript{2}; Eunyoung Park\textsuperscript{2}; Jaeyeon Kim\textsuperscript{2}; Facundo M. Fernandez\textsuperscript{2}; \textsuperscript{1}School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia; \textsuperscript{2}Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN; \textsuperscript{3}Indiana University Melvin & Bren Simon Cancer Center, Indianapolis, IN

Metabolomic mapping of mouse thymus with Imaging Mass Microscope as a whole animal model; Yudai Tsuji\textsuperscript{1}; Shinichi Yamaguchi\textsuperscript{2}; Takashi Yamamoto\textsuperscript{2}; Tomoyuki Nakamura\textsuperscript{2}; Masaya Ikegawa\textsuperscript{1}; \textsuperscript{1}Doshisha University, Kyotanabe, Japan; \textsuperscript{2}Shimadzu Corporation, Kyoto, Japan; \textsuperscript{3}Kansai Medical University, Hirakata, Japan

Investigating the interactions of the first 17 residues of Huntington protein with lipid vesicles using ESI-MS experiments and MD simulations; Ahmad Kiani Karanj\textsuperscript{1}; Maryssa Beasely\textsuperscript{1}; Daud Sharif\textsuperscript{1}; Ali Ranjarban\textsuperscript{1}; Justin Legleiter\textsuperscript{1}; Stephen J Valentine\textsuperscript{1}; \textsuperscript{1}West Virginia University, Morgantown, WV

Quality assessment of MALDI TOF and ion mobility MSI data based on mass defect and CCS filtering; Tobias Boskamp\textsuperscript{1, 2}; Rita Casadonte\textsuperscript{1}; Lena Hauberg-Lotte\textsuperscript{2}; Janina Oetjen\textsuperscript{2}; Alice Ly\textsuperscript{2}; Sören-Oliver Deininger\textsuperscript{1}; Jan H. Kobarg\textsuperscript{1}; Richard Drake\textsuperscript{1}; Jörg Kriegsmann\textsuperscript{3}; Peter Maass\textsuperscript{2}; Dennis Trede\textsuperscript{1}; \textsuperscript{1}Bruker Daltonik GmbH, Bremen, Germany; \textsuperscript{2}University of Bremen, Bremen, Germany; \textsuperscript{3}Proteopath GmbH, Trier, Germany; \textsuperscript{4}Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim Technical University, Mannheim, Germany
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**ThP 265** Development of data processing tools for conformational mass spectrometry imaging; Emma K Sisley1; Iain B Styles1; Helen J Cooper3; 1University of Birmingham, Birmingham, United Kingdom

**ThP 266** Intact mass spectrum imaging of human non-alcoholic fatty liver disease on an orbitrap eclipse using a cylindrical FAIMS DEVICE; James W. Hughes1; Iain B. Styles1; Patricia F. Lalor1; Helen J. Cooper1; 1University of Birmingham, Birmingham, United Kingdom

**ThP 267** A multi-layered desorption electrospray ionisation (DESI) mass spectrometry imaging workflow for fully annotated datasets; Emrys A Jones1; Praveen Harapanahalli2; Emmy Hoyes3; Keith Richardson3; Michael Morris3; 1Waters Corporation, Wilmslow, United Kingdom

**ThP 268** Using high abundance proteins as guides for fast and effective peptide/protein identification from metaproteomic data; Moses H Stamboulian1; Sujuan Li1; Yuzhen Ye1; 1Indiana University, Bloomington, IN

**ThP 269** Feature Engineering Guided by Matrix Effects for Mass Spectrometry Imaging Segmentation and Co-localization; Hang Hu1; Ruichuan Yin1; Jyothisa Padmakumar Bindu1; Julia Laskin1; 1Purdue 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 Föll1; Veronika Volkmann1; Kathrin Enderle-Ammour2; Peter Bronsert1, 2, 3; Oliver Schilling1, 2; 1Institute of Surgical Pathology, Medical Center, Freiburg University, Freiburg, Germany; 2German Cancer Consortium (DKTK) and Cancer Research Center (DKFZ), Freiburg, Germany; 3Tumorbank 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 Zou1; Pengchun Yu2; Xiang Tian1; Jie Zhu2; Zhibo Yang1; 1University of Oklahoma, Norman, OK; 2Oklahoma Medical Research Foundation, Oklahoma City, OK; 3Astrazeneca, Gaithersburg, MD

**ThP 272** Structure-preserving and perceptually-consistent approach for visualization of mass-spectrometric imaging datasets; Anastasia Sarycheva1; Anton Grigoryev1, 2; Dmitry Sidorchuk2; Gleb Vladimirov1; Yury Kostyukevich1; Eugene (evgeny) Nikolaev1; 1Skolkovo institute of science and technology, Moscow, Russia; 2Kharkiev 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; Wangjiu Zhang1, 2; Nico Verbeeck1, 2; Thomas Moerman2; Etienne Waelden2; Marc Claesen1, 2; Bart De Moor1; 1KU Leuven, ESAT-STADIUS, Leuven, Belgium; 2Aspect Analytics NV, Genk, Belgium; 3KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium

**ThP 274** Deep multiple instance learning classifies subepithelial locations in mass spectrometry images from tissue-level annotations; Dan Guo1; Melanie Christine Föll2; Veronika Volkmann2; Kathrin Enderle-Ammour2; Peter Bronsert1, 2; Oliver Schilling2; Olga Vitek1; 1Northeastern University, Boston, MA; 2University of Freiburg, Freiburg, Germany; 3German 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 Shedlock1; Tyler Bielinski1; Nolan K Mclaughlin1; Jason Graham1; Katherine A. Stumpo1; 1University of Scranton, Scranton, PA

**ThP 276** Towards nanoscale molecular mass spectrometry imaging via physically constrained machine learning on coregistered multimodal data; Nickolay Borodinov1; Matthias Lorenz1, 2; Dustin Klein2, 3; Jeffrey M Spraggs4, 5, 6, 7; Anton leviev1; 1Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; 2University of Tennessee Knoxville, Knoxville, TN; 3Vanderbilt University, Department of Biochemistry, Nashville, TN; 4Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 5Vanderbilt University Department of Chemistry, Nashville, TN

**ThP 277** Automatic detection and identification of drug metabolites in MSI datasets; Fabien Pameiard1; Anas Carfache1; Mathieu Gaudin1; Rima Ait Belkacem1; David Bonnel2; Jonathan Stauber2; 1ImaBiotech, Loos, France; 2ImaBiotech, Billerica, Massachusetts

**INFORMANTS: PEPTIDE ID AND QUANTIFICATION**

**ThP 278** Concurrent Glycopeptide Identification from multiple related LC-MS/MS datasets by using spectra clustering; Rui Zhang1; Sujuan Li1; Lei Wang1; Jinhui Zhu2; Yehia Mechref3; David M Lubman4; Haixu Tang1; 1Indiana University, Bloomington, IN; 2University of Michigan, School of Medicine, Rogel Cancer Center, Ann Arbor, Michigan; 3Texas Tech University, Lubbock, Texas; 4University of Michiganan, Ann Arbor, MI

**ThP 279** Trypsin - a Tired Workhorse? The Selectivity of Atypical Cleavages by Trypsin; Meghan Burke1; Yuxue Liang1; Stephen E. Stein1; 1National 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 Poudel1; Yuxin Li2; Junmin Peng2, 3; 1Departments of Structural Biology and
Breaking the logjam: fast peptide identification and quantification in timsTOF PASEF data; Fengchao Yu1; Sarah E. Haynes1; Guo Ci Teo1; Dmitry M. Avtonomov1; Andy T. Kong1; Felipe Da Veiga Leprevost1; Alexey I. Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

PASER: Parallel Database Search Engine in Real-Time; Robin Park1; Patrick Garrett1; Michael Krause2; Sven Brehmer2; Titus Jung1; Peter Huffnagel2; Christopher Adams2; Casimir Bamberger1; Jolene Diedrich1; John Robert Yates III1; 1The Scripps Research Institute, La Jolla, CA; 2Bruker, Bremen, Germany

An extension of Mass++ ver.4, a data viewer, for proteome analysis; Satoshi Tanaka1; Masaki Murase2; Masaki Kato2; Tsuyoshi Tabata1; Maiko Kusano1; Shin Kawan1; Susumu Goto5; Yasushi Ishihama2; Akiyasu C. Yoshizawa2; 1Trans-JT, Kaminokawa-machi, Tochigi Pref., Japan; 2Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; 3Res. Inst. of Environ. Med., Nagoya Univ., Nagoya, Japan; 4Toyama Intl. Univ., Toyama, Japan; 5DBCLS, DS, ROIS, Kashiwa, Japan

A Machine-Learning-Combined Scoring Method for Peptide Feature Detection from LC-MS; Xiangyu Zeng1; Bin Ma1; Shenheng Guan2; 1University of Waterloo, Waterloo, ON; 2University of California, Los Angeles, Los Angeles, CA

PointNovo: instrument-resolution-independent de novo peptide sequencing with deep learning; Rui Qiao1; Ngoc Hieu Tran2; Lei Xin2; Xin Chen2; Baozhen Shan1; Ming Li1; Ali Ghodsi1; 1University of Waterloo, Waterloo, ON; 2Bioinformatic Solutions Incorporation, Waterloo, Ontario

Machine learning-based spectral filtering tool for processing peptide mass spectra; Krishna Anapindi1, 2; Yuxuan Xie1, 2; Jonathan V Sweedler1, 2; 1University of Illinois at Urbana-Champaign, Urbana, IL; 2Beckman Institute, Urbana, IL

Deep learning-derived evaluation metrics for benchmarking computational pipelines for the analysis of large-scale phosphoproteomics datasets; Wen Jiang1; Kai Li1; Bo Wen1; Bing Zhang1; 1Baylor College of Medicine, Houston, TX

Rapid Total Search: Peptide Identification in 200 Million Proteins with Unrestricted Modifications and Nonspecific Digestion; Qixin Liu1; Noah Reinhardt1; Bin Ma1; 1Rapid Novor inc, Kitchener, ON; 2Rapid Novor Inc, Waterloo, ON; 3University of Waterloo, Waterloo, ON

PASEF and Bolt: enabling comprehensive analysis via high MS/MS acquisition speed and MS/MS sequencing through vast protein databases in minutes; Amol Prakash1; Swetaketu Majumder1; Jiefei Tong2; Shenheng Guan1; Matt Willetts1; Bin Ma1; Tharan Srikumar2; Michael F. Moran2; 1Optys Tech Corporation, Shrewsbury, MA; 2Sick Kids Research Center, Toronto, M5G1X8; 3University of Waterloo, Waterloo, ON; 4Bruker Scientific LLC, Billerica, MA; 5Bruker Ltd, Milton, L9T 6P4

Filtering and optimization of peptide tandem mass spectral libraries; Sergey Sheetlin1; Guanghui Wang1; Dmitrii V. Tchekhovskoi1; Zheng Zhang1; Stephen E. Stein1; 1NIST, Gaithersburg, MD

A proteogenomics pipeline for identifying sample-specific proteoforms by combining RNA-Seq and top-down mass spectrometry; Wenrong Chen1; Xiaowen Liu1; 1Indiana University Purdue University Indianapolis, Indianapolis, IN

MS Amanda goes West: Integrating a search engine into Skyline; Viktoria Dorfer1; Marina Strobl1; Nicholas Shulman2; Matthew C Chambers2; Michael J MacCoss2; Brendan Maclean2; 1Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria; 2Department of Genome Sciences, University of Washington, Seattle, WA

Separating the wheat from the chaff: Prediction-assisted rescoring; Siegfried Gusslat1; Tobias Schmidt2; Michael Graber1; Florian Seefried1; Carmen Paschke1; Kai Fritzemeier2; David M Horn3; Bernard Delanghe3; Daniel P Zolg4; Mathias Wilhelm2; Bernhard Kuster2; Martin Heinrich Frejno1; 1msAId GmbH, Garching, Germany; 2TU Munich, Freising, Germany; 3Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; 4Thermo Fisher Scientific, San Jose, CA

The good, the bad and the ugly: Peptide IDs you will encounter; Siegfried Gusslat1; Tobias Schmidt2; Michael Graber1; Florian Seefried1; David M Horn3; Bernard Delanghe3; Daniel P Zolg4; Mathias Wilhelm2; Bernhard Kuster2; Martin Heinrich Frejno1; 1msAId GmbH, Garching, Germany; 2TU Munich, Freising, Germany; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

Comprehensive analysis of the intermolecular associations of peanut proteins by SEC coupled with offline bottom-up MS; Abigail S Burrows1; Justin T Marsh1; Philip E Johnson1; 1University of Nebraska - Lincoln, Lincoln, NE
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ThP 307 A new algorithm for HDMS data analysis with deep proteome coverage; Zia Rahman1; Leroy B Martin II2; Susan Slade2; Di Wang1; Weiwu Chen1; Baozhen Shan1; 1Bioinformatics Solutions Inc, Waterloo, ON; 2Waters Corporation, Milford, Massachusetts; 3Waters Corporation, Wilmslow, United Kingdom

ThP 298 Identifying genetically variant peptides in cancer samples by the NIST hybrid spectral library search; Guanghui Wang1; Meghan C. Burke1; Sergey L. Sheetlin1; Yuri A. Mirokhin1; Dmitrii V. Tchekhovskoi1; Stephen E. Stein1; 1NIST, Gaithersburg, MD

ThP 299 Interactive Spectrum Validator as an inter-resource tool for fragment ion spectrum comparison between experimental and (predicted) reference spectra; Tobias Schmidt1; Patroklos Samaras1; Viktoria Dorfer2; Christian Panse1; Tobias Kockmann1; Leon Bichmann1; Bart Van Puyvelde1; Yasset Perez-Riverol6; Eric W. Deutsch1; Wout Bittremieux1; Bernhard Kuster1; Mathias Wilhelm1; 1Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 2Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria; 3Functional Genomics Center (ETH), Zurich, Switzerland; 4Applied Bioinformatics, Tübingen, Germany; 5Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium; 6European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Hinxton, United Kingdom; 7Institute For Systems Biology, Seattle, WA; 8University 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 Whitworth1; Katherine B Henke1; Robert J Millikin1; Hemanth Potluri2; Mark Scal1; Brian L Frey1; Michael R. Shortreed1; Douglas G Mcneel1; Lloyd M Smith1; 1University of Wisconsin-Madison, Madison, Wisconsin; 2University of Wisconsin School of Medicine and Public Health, Madison, WI; 3University of Wisconsin Carbone Cancer Center, Madison, WI

ThP 301 Restricting classifier training datasets improves error rate estimation when searching highly-specific libraries; Seth Just1; Brendan Maclean1; Lukas Käll2; Hannes Röst3; Brian Searle1, 5; 1Proteome Software, Portland, OR; 2University of Washington, Seattle, WA; 3Royal Institute of Technology - KTH, Solna, Sweden; 4University of Toronto, Toronto, ON; 5Institute 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. Raczewski1; Bo Wen1; James E. Johnson1; Ray Sajulga1; Qiyuan Han1; Praveen Kumar1; Pratik Dilip Jagtap1; Bing Zhang2; Natalia Tretyakova1; Timothy J Griffin1; 1University of Minnesota at Twin Cities, Minneapolis, MN; 2Baylor College of Medicine, Houston, TX

ThP 303 Quality Control of Results from Searchable Spectral Archive; Long Wu1; Henry Lam1; 1The 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 Wertz1; Nuno Bandeira1; 1University 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 Wen1; Kai Li1; Yun Zhang1; Bing Zhang1; 1Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX

ThP 307 Clustering of label-free quantitation data: a quantitation-first approach; Matthew The1, 2; Lukas Käll1; 1Royal Institute of Technology - KTH, Solna, Sweden; 2TU Munich, Munich, Germany

ThP 308 New functionality for the Trans-Proteomic Pipeline: tools for the analysis of proteomics data; Luis Mendoza1; David Shteynberg1; Michael Hoopmann1; Henry Lam1; Jimmy K Eng1; Eric W. Deutsch1; Robert L. Moritz1; 1Institute For Systems Biology, Seattle, WA; 2Hong Kong University of Science and Technology, Hong Kong, China; 3University of Washington, Seattle, WA

ThP 309 Compliant-Ready Intact Biotherapeutic Protein Quantitation Using Reconstructed Masses; Kerstin Pohl1; Wenyiing Jian1; Naidong Weng1; Yihan Li1; Ji Jiang1; Xu Guo1; Vanaja Raguvan1; Lei Xiong1; 1ScieX, Framingham, MA; 2Jansen R&D LLC., Spring House, PA; 3SCIEX, Redwood Shores, CA; 4SCIEX, 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 Baker1; Juan A. Oses2; Bing Gao2; Robert J. Chalkley2; 1UCSF, Rokietnica, Poland; 2UCSF, San Francisco, CA

ThP 311 Proteomic analysis of multiple neuroanatomical regions of Normal Human Brain: a database and community resource for neuroscience research; Deepartup Biswas1; Chetanya Gupta1; Sanjyot Shenoy1; P. Athithyan1; Susmita Ghosh1; Sudeep Roy1; Sanjeeva Srivastava1; 1IIT Bombay, Mumbai, India

ThP 313 Proceed with caution: Considerations for Protein Inference and Quantitation in Metaproteomics; Samantha L. Peters1, 2; Payal Chirania1, 2; Paul E. Abraham1, 2; Richard J. Giannone1, 2; Robert L. Hettich1, 2; 1Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; 2University of Tennessee Knoxville, Knoxville, TN
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ThP 314  TMT-Pro 16-plex labeling and unsupervised clustering for analysis of organellar proteome dynamics; Nicholas Carruthers1; Kezhong Zhang1; Paul M. Stemmer1; 1Wayne State University, Detroit, MI

ThP 315  De Novo Sequencing with Twister: Expanding Opportunities; Kira Vyatkina; Alferov University, St Petersburg, Russia

ThP 316  Integration of MSstatsTMT into Proteome Discoverer using the Scripting Node; David M. Horn1; Ting Huang2; Meena Cho2; Olga Vitek2; Rosa I. Viner1; Frank Berg2; Kai Fritzemeier3; Carmen Paschke; 1Thermo Fisher Scientific, San Jose, CA; 2Northwestern University, Boston, MA; 3Thermo 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 Avtonomov1; Fengchao Yu1; Guo Ci Teo1; Felipe Da Veiga Leprevost1; Sarah E. Haynes1; Hui-Yin Chang1; Daniel J. Geiszler1; Daniel A. Polasky1; Alexey I. Nesvizhskii1; 1University 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; Robert Millikin1; Michael R. Shortreed1; Mark Scalf1; Lloyd M. Smith1; 1University of Wisconsin Madison, Madison, WI

ThP 319  A new algorithm for FAIMS data analysis with accurate in-depth quantitative profiling; Zia Rahman1; Yandong Zhu2; Kassim Santone2; Zheng Chen2; Bernard Delange3; Baozhen Shan2; 1Bioinformatics Solutions Inc, Waterloo, ON; 2Bioinformatics Solutions Inc., Waterloo, ON; 3Thermo Fisher Scientific, Cambridge, MA

ThP 320  MealTime-MS: A machine learning-guided real-time mass spectrometry analysis for protein identification and efficient dynamic exclusion; Yun-En Chung1; Alexander R. Pelletier1; Zhibin Ning1; Nora Wong1; Daniel Figey1; Mathieu Lavallée-Adam1; 1University of Ottawa, Ottawa, ON

INSTRUMENTATION: NEW DEVELOPMENTS IN ION DETECTION

ThP 321  A fast ultra-low noise current amplifier with linear dynamic range from femtoamperes to nanoamperes; Ansgar T. Kirk1; Cornelius Wendt1; Stefan Zimmermann1; 1Leibniz 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; Li-Xue Jiang1; Mark E. Bier1; 1Carnegie Mellon University, Pittsburgh, PA

ThP 323  A Discrete-Dynode Detector for Quadrupole RGA Applications; Aditya Wakhe1; Peter Raffin1; Sid Sondur1; Toby Shanley1; Scott Morgan1; 1Adapta Solutions, Sydney, Australia

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS

ThP 324  A Robust C-Trap Ion Injection Method Incorporating Electrodynamic Squeezing; Hamish Stewart1; Ralf Hartmer1; Christian Hock1; Amelia Peterson1; Eric Wapelhorst1; Alexander Makarov1; 1Thermo Fisher Scientific, Bremen, Germany

ThP 325  Increasing the resolving power in a High Field Cassinian ion trap; Björn Raupers1; Hana Medhat2; Frank Gunzer2; Tassilo Muskat1; Jurgen Grottemeyer1; 1Christian-Albrechts-Univ, Kiel, Germany; 2German 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; Peter T. A. Reilly1; Adam P. Huntley1; Margaret E. Reece1; 1Washington 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 Bracewell1; Liam Duffy1; 1University of North Carolina Greensboro, Greensboro, NC

ThP 328  Electrospray Ionization Time-of-Flight Mass Spectrometry Using Constant Momentum Acceleration; Christopher J Brais1; Eric T Jensen1; Steven J Ray1; 1University at Buffalo, SUNY, Buffalo, NY

ThP 329  Combinatorial improvement in spectral acquisition rates with harmonic signal and MS array ICR detectors; Sung-Gun Park1; Jared P. Mohr1; Gordon A. Anderson2; James E Bruce1; 1University of Washington, Seattle, WA; 2GAA Custom Engineering, LLC., Benton, WA

ThP 330  Innovations in MS-MS: Development of a Versatile Q-ToF Molecular Beam Mass Spectrometer; Greg Thier1; Steven M Rowland1; Brian Regel1; 1Exelr CMS, Pittsburgh, PA; 2National Renewable Energy Laboratory, Golden, CO

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**Ion Mobility-Mass Spectrometry and Ozone-Induced Cleavage of Endocyclic C=C Bonds to Separate Isomeric Prostaglandins**; Kristie Baker1; Samuel W Maddox1; Robert H Fraser-Caris1; Christopher D. Chouinard1; 1Florida Institute Of Technology, Melbourne, FL

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**Absolute quantification of proteins by electrospray-differential mobility analysis-condensation particle counter**; Wei Mi1; Zhishang Hu1; Yang Liu2; 1National institute of metrology, China, Beijing, China; 2Beijing 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 Sarbu1; VuKelic Zeljka1; David E. Clemmer1; Alina D. Zamfir1; 1National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; 2Indiana University, Bloomington, IN; 3Natl Inst, Electrochemistry & Condensed Matter, Timisoara, Romania

ThP 334  
**Identification and Localization of Isomers in Eye Lens Crystallin Peptides Using TWIM-MS**; Hoi Ting Wu1; Ryan R. Julian1; 1University 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 Guo1; Gonyu Li1; Lingjun Li1; 1University of Wisconsin-Madison, Madison, Wisconsin

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**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 Green1; Keith Richardson1; Brandon T. Ruotolo2; Daniel A. Polasky2; Heidi Gastall1; 1Waters Corporation, Wilmslow, United Kingdom; 2University of Michigan, Ann Arbor

ThP 337  
**Utilizing U-Shaped Mobility Analyzer (UMA) for High Performance Bio-molecular Analysis**; Ran Qiu1; Keke Wang1; Xiaoliang Zhang1; Wenjian Sun1; 1Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China

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**Deep dive into timsTOF data with MSFragger**; Sarah E. Haynes1; Fengchao Yu1; Guo Ci Teo1; Felipe Da Veiga Leprevost1; Dmitry M. Avtonomov1; Alexey I. Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

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**Post-ionization mobility separation for MALDI based analysis of isomeric cannabinoids in plant samples**; Arne Behrens1; Corrina Henkel1; Uwe Karst1; 1Westfälische Wilhelms-Universität Münster, Münster, Germany; 2Bruker Daltonik GmbH, Bremen, Germany

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**A Novel In-Source Ion Fragmentation Device for Complementary Mass Spectrometry**; Andrzej Balinski1; Jaqueline A. Picache1; Ruwan T. Kurulugama2; Emanuel Zlibut1; Jody C. May1; John C. Fjeldsted2; John A. McLean1; 1Waters Corporation, Milford, Massachusetts; 2Bruker Daltonics, Billerica, MA

ThP 341  
**Structural Differentiation of Buspirone Hydroxy Metabolites with Cyclic Ion Mobility Spectrometry**; Lauren Mullin1; Mark D. Wrona1; Martin Palmer2; Emma Marsden-Edwards2; Robert Plumb1; 1Waters Corporation, Milford, Massachusetts; 2Waters Corporation, Wilmslow, United Kingdom

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**Structural Analysis of the Glycoprotein Complex Avidin by Tandem-Trapped Ion Mobility Spectrometry**; Fanny C. Liu1; Tyler C Cropley1; Valentina R. Angarita1; Wessley Ferguson1; Mark E. Ridgeway2; Melvin A. Park2; Christian Bleiholder1; 1Florida State University, Tallahassee, FL; 2Bruker Daltonics, Billerica, MA

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**Ion mobility separation in a TIMS-TOF PASEF acquisition method decreases spectral complexity**; Joshua Charkow1; Annie Ha1; Tom W Ouellette1; Aparna Srinivasan1; Hannes Rost1; 1University of Toronto, Toronto, ON

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**Characterization of API impurities and degradation products by ion mobility LC-timsTOF Pro with parallel accumulation serial fragmentation (PASEF)**; Zuyun (peel) Huang1; Lilly Huang1; Song Sun1; Xuejun Peng2; 1SYN Pharmatech, Guelph, ON; 2Bruker Daltonics Inc., San Jose, CA

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**The Potential of Cyclic-Ion-Mobility Mass-Spectrometry for the Separation of Steroid Isomers: Application in Food Fraud and Safety**; Eleanor Riches1; Nicola Dreolin1; Maykel Hernandez-Mesa1; Gaud Dervilly2; Bruno Le Bizec2; 1Waters Corporation, Wilmslow, United Kingdom; 2LABERCA Oniris INRAE, Nantes, France

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**Cyclic ion mobility-spectrometry (cIMS) deciphers disulphide bridge pairing in Complementary-Determining Regions (CDRs) of an IgG4 monoclonal antibody**; Hélène Diemer1; Thomas Botzanowski1; Dale Cooper-Shepherd2; Elsa Wagner-Rousset1; Evolène Designière1; Olivier Colas1; Guillaume Béchade1; Oscar Hernandez-Alba1; Alain Beck3; Sarah Cianférani1; 1Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; 2Waters Corporation, Wilmslow, United Kingdom; 3IRPF - Centre d’Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France

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**Comparison of ion mobility mass spectrometry using direct injections or chromatography in quantitative metabolomics of Rooibos and Honey bush tea**; Maria A Stander1; Keabetswe Masike2; Dalene De Beer3, 4; Andre De Villiers5; 1Stellenbosch University, Stellenbosch, South Africa; 2Stellenbosch University, Department of Biochemistry, Stellenbosch, South Africa; 3ARC Infruteic-Nietvoorbij, Stellenbosch, South Africa; 4Stellenbosch University, Stellenbosch, South Africa; 5Stellenbosch University, Stellenbosch, South Africa
Short abstract, Poster PDF, and optional presentation video will be included.

**University, Stellenbosch, South Africa**; **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 Hooshfar1; Kara L Lynch1; \(^1\)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 Morre1; Rony Koluda1; Dr. Claudia Susanne Maier1; \(^1\)Oregon State University, Corvallis, OR

**ThP 350** Profiling of the Known-Unknowns Passiflora Complement by Liquid Chromatography - Ion Mobility - Mass Spectrometry; Michael Mccullagh1; Jeff Goshawk1; Russell J Mortishire-Smith1; Cintia AM Pereira2; Janete H Yariwak3; Johannes P.C. Vissers1; \(^1\)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

ThP 351 Zwitterionic HILIC chromatography - tandem mass spectrometry quantification of acyl carnitines and lysophosphatidic acids: Key metabolites in lipid metabolism; Natalie Dauro1; Kathleen Smith1; David Beebe1; Kenneth Kelly1; Gang Xing1; Trenton Ross1; Min Wan1; Michelle Cas Quinn1; 1Pfizer, Cambridge, MA

ThP 352 Quantitative Analysis of Cardiolipins by Tandem LC/MS; Chen Chen He1; Thekkelavyczke M. Rajendiran2; Subramaniam Pennathur1; 1University of Michigan, School of Medicine, Internal Medicine – Nephrology, Ann Arbor, Michigan; 2University 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 Schoeny1; Evelyn Rample1;1, 2, 3, Felina Hildebrand1; Olivia Zach1; Gerrit Hermann1, 4; Gunda Koellensperger1, 2, 3, 4; University of Vienna, Department of Analytical Chemistry, Vienna, Austria; 2Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria; 3Chemistry meets Microbiology, University of Vienna, Vienna, Austria; 4Isotope Solutions, Vienna, Austria

ThP 354 The Blood Plasma Lipidome: distinct molecular signatures delineate metabolic health and perturbations in a cross-sectional human cohort; Si Wu1; Daniel Hornburg1; Gavin McAllister Traber1; Baolong Su2; Tejaswini Mishra1; Wenyu Zhou1; Kevin Contrepois1; Sophia Miryam Schüssler-Fiorenza Rose1; Monika Avina1; Kevin Williams2; Michael Snyder1; 1Stanford University, Palo Alto, CA; 2UCLA, Los Angeles, CA

ThP 355 Lipidome-specific features of matrix-bound nanovesicles define their anti-inflammatory and macrophage M2-polarization capacities; Yulia Tyurina1; Vladimir A Tyurin1; George S Hussey1; Madeline C Cramer1; Yulia Tyurina1; Vladimir A Tyurin1; George S Hussey1; Madeline C Cramer1; 1University of Michigan, School of Medicine, Internal Medicine – Nephrology, Ann Arbor, Michigan; 2University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan

ThP 356 Rapid and quantitative of phospholipid molecular species in plasma based on magnetic solid-phase extraction by MnFe2O4 nanoparticles coupled with LC-HR/MS/MS; Liangfei Cao1; Jiaxin Feng1; Qingyuan Hu1; Xu Zhao1; Zheng Ouyang1; Xiaoxiao Ma1; 1University of Florida, Gainesville, FL

ThP 357 Genome-wide study of the human lipidome and links to cardiovascular disease risk; Corey Giles1; Gemma Cadby2; 3; Kevin Huynh1; Natalie A Mellett1; Gabriol Olshansky1; Alexander Smith1; Anh Nguyen1; Michael Inouye1; 1National Chung-Hsing University, Taichung, Taiwan

ThP 358 Stearoyl CoA desaturase regulates the composition of lipid C=C location isomers; Simin Cheng1; Wenbo Cao1; Jixian Feng1; Qingyuan Hu1; Xu Zhao1; Zheng Ouyang1; Xiaoxiao Ma1; 1Tsinghua University, Beijing, China

ThP 359 Accumulation of Lysophospholipids in DDE/Dieldrin Treated Largemouth Bass (Micropterus salmoides) Liver Quantified by Targeted Mass Spectrometry; Mohammad-Zaman Nouri1; Kevin Kroll1; Nancy Denslow1; 1University of Florida, Gainesville, FL

ThP 360 Sensitive and Comprehensive Lipid Mediator Analysis using Advanced Scheduled MRM with Polarity Switching and QTRAP Enhanced Product Ion Scanning; Paul C Norris1; Santosh Kapil Kumar Gorti1; Paul C Norris1; Santosh Kapil Kumar Gorti1; 1University of Pittsburgh, Pittsburgh, PA; 2IM Sechenov Roskamp Institute, Sarasota, FL

ThP 361 Method development of high-throughput eicosanoid profiling for micro-sampling plasma; Minako Yamada1; Naoko Nagano1; Tatsuro Nakamura2; Takahisa Murata2; Roderick Roper1; 1The University of Tokyo, Bunkyo-ku, Japan; 2Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria; 3Chemistry meets Microbiology, University of Vienna, Vienna, Austria

ThP 362 Genome-wide study of the human lipidome and links to cardiovascular disease risk; Gemma Cadby1; Kevin Huynh1; Natalie A Mellett1; Gabriol Olshansky1; Alexander Smith1; Anh Nguyen1; Michael Inouye1; 1National Chung-Hsing University, Taichung, Taiwan

ThP 363 A validated multiplexed quantitative global molecular lipidomics method with extended coverage for routine use; Renz N Zhang1; Nathan Hatcher1; Komal Hatton1; Kevin P. Bateman1; Kim Ekoos2; 1Merk & Co., Inc., West Point, PA; 2Lipidomics Consulting Ltd, Vantaa, Finland

ThP 364 Development of Extraction Protocol for Telocinobufagin and Investigation of its Enzymatic Hydrolysis by Paraoxonase-1 using HPLC and MS; Sabitha Lachman1; Chrysan Joy Mohammed1; David Baill-Rodriguez1; Steven T. Haller1; David J. Kennedy1; Dragana Isailovic1; 1University of Toledo, Toledo, OH; 2University of Toledo, Toledo, Ohio

ThP 365 Probing the Mechanism of Zika Infection/Replication Using Lipidomics And Proteomics Analyses; Roderick G. Davis1; Roskamp Institute, Sarasota, FL

ThP 366 Investigation of the Sulfo-Phospho-Vanillin Assay to Measure Total Lipid Content for Uniform Loading in Quantitative Lipidomic LC-MS/MS Analyses; Laura Bailey1; Kari Basso1; 1University of Florida Department of Chemistry, Gainesville, FL

ThP 367 Probing the Mechanism of Zika Infection/Replication Using Lipidomics And Proteomics Analyses; Roderick G. Davis1; Roskamp Institute, Sarasota, FL

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**ThP 368**

**Untargeted LC-MS/MS-based metabolic phenotyping applied to the CD248 knock out mouse model:**

Neil J. Loftus1; Emily Armitage1; Alan Barnes1; Janak Bechara2; Ed Rainger3; Matthew Harrison4; Ian D. Wilson5; Christopher D. Buckley6; Amy J. Naylor2; 1Shimadzu MS/BU, Manchester, United Kingdom; 2Rheumatology Research Group, Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; 3Institute of Cardiovascular Sciences, University of Birmingham, Birmingham, United Kingdom; 4Dept 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 Kamal1; Kevin Zhu1; Lina Abi Mosleh1; Madison Roberts1; Gul Nowshad1; Mohamad Ammar Ayass3; 1Ayass BioScience, LLC, Frisco, TX

**ThP 370**

**Metabolomics and lipidomics study of plasma from ischemic stroke patients for differentiation of subtypes of ischemic stroke:**

Jianying Wang1; Zhongping Yao1; 1The 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. Amara1; Danthasinghe Weduge Badrajee Piyarathna1; Roni J. Bollag2; Martha K. Terns3; Lotan Yal1; Arun Sreekumar1; Shyam M. Kavuri1; Nagireddy Puturi1; 1Baylor College of Medicine, Houston, TX; 2Augusta University, Augusta, GA; 3UTSW, Dallas

**ThP 372**

**Quantification of membrane lipids as biomarkers of aging relevant to Alzheimer’s disease:**

Gabriela Dovtelova1; Petr Telensky2; Lukas Opalka2; Jana Klanova2; Ales Hampi2; Jiri Damborsky1; Zdenek Spacil4; 1Masaryk University, Brno, Czech Republic; 2Charles University, Prague, Czech Republic; 3Charles University, Hradec Kralove, Czech Republic; 4Masaryk 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. Richard1; Constanze A. Sobsey1; Noor Mady2; René P. Zahedi2; Robert Thomas Jagoe3, 4, 5; Christoph H. Borchers1, 3, 4; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Peter Brodie Lung Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4Dept 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 Vaswani1, 2; Dr. Armando Alcazar Magana1, 2; Dr. Eric Zimmermann1; Dr. Jaishankar Raman3, 4, 5; Dr. Claudia Susanne Maijer1, 2; 1Oregon State University, Corvallis, OR; 2Oregon Health & Science University, Portland, Oregon; 3St Vincent’s Hospitals, Melbourne University, Melbourne, Australia; 4Deakin University, Geelong & Melbourne, Melbourne, Australia

**ThP 375**

**Metabolomics in precision medicine – are common software utilities and databases ready for its application?**

Stephen Barnes1; Ceren Yarar1; Jia Li1; Landon S Wilson1; Taylor F. Berryhill1; Rebecca Howell1; Amie Mclain1; 1University of Alabama at Birmingham, Birmingham, AL

**ThP 376**

**Metabolic analysis of HIV-Associated Neuropathogenesis And Prodromal Alzheimer’s Disease:**

Emmanuel Elijah1; Nikesh Kumar2; Thomas Vollbrecht3; Alan K. Jarmusch4; Fernando Vargas4; Scott Letendre5; Kathiiein Fisch1; Douglas Galasko2; Robert K Heaton3; Pieter C. Dorrestein4; Michelli Oliveira5; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Rheumatology Research Group, Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; 3Institute of Cardiovascular Sciences, University of Birmingham, Birmingham, United Kingdom; 4Dept Metabolism, Digestion and Reproduction, Imperial College, London, United Kingdom

**ThP 376**

**Untargeted Spatial Lipidomics of Colon Carcinoma Spheroids:**

Fernando Tobias1; Amanda B. Hummon1; 1The Ohio State University, Columbus, OH
ThP 381 Exploring Bacterial Metabolome Alterations Mediated by Genetic Mutations; Eric D Tague1; Sven Hackbusch1; 1Thermo Fisher Scientific, San Jose, CA

ThP 382 Sphingolipid variations between hypertensive and normotensive patients elucidated by Magnetic Resonance Mass Spectrometry; Eduardo Sommella1; Fabrizio Mercoli1; Matthias Witt2; Jochen Friedrich2; Paola Di Pietro1; Pietro Campiglia1; 1University of Salerno, Fisciano, Italy; 2Bruker Daltonik GmbH, Bremen, Germany

ThP 383 4-dimensional annotation of Metabolomics features: CCS values as an additional source for higher confidence; Ulinko Schweiger-Hufnagel1; Matthias Szesny1; Aiko Barsch1; Melvin Gay2; Torben Kimhofer2; Joel Gunner1; Luke Whiley1; Jeremy Nicholson2; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker Pty. LTD., Australia, Preston, Australia; 3Murdock 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 Sarma1, 2; Brittany L Marshall2, 3; Yang Liu2, 4; Michelle J Farrington2, 3; Jiude Mao2, 8; Nathan J Bivens2, 5; Zhentian Lei1, 2, 6; Lloyd W Sumner1, 2, 6; Trupti Joshi2, 4, 7; Cheryl S Rosenfeld2, 4, 8, 9; 1Metabolomics Center, University of Missouri, Columbia, MO; 2Bond Life Sciences Center, University of Missouri, Columbia, MO; 3Biomedical Sciences, University of Missouri, Columbia, MO; 4MU Data Science and Informatics Institute, Columbia, MO; 5DNA Core Facility, University of Missouri, Columbia, MO; 6Department of Biochemistry, University of Missouri, Columbia, MO; 7Department of Health Management and Informatics, University of Missouri, Columbia, MO; 8Thompson Center for Autism and Neurobehavioral Disorders, University of Missouri, Columbia, MO; 9Genetic Area Program, University of Missouri, Columbia, MO

ThP 385 Metabolite Profiling of Experimental Cutaneous Leishmaniasis Lesions Demonstrates Significant Perturbations in Tissue Phospholipids; Adwita R. Parab1; Diane Thomas2; Sharon Lostracco-Johnson2; Jair L Siqueira-Neto2; James Mckerrow2; Pieter C. Dorrestein3; 1The Ohio State University, Columbus, OH; 2The Pennsylvania State University, University Park, PA; 3Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; 4Collaborative Mass Spectrometry Innovation Center, University of California San Diego, La Jolla, California; 5Department of Medicine, Washington University in St. Louis, St. Louis, MO; 6Department of Chemistry, Washington University in St. Louis, St. Louis, MO; 7Department of Biochemistry, University of Oklahoma, Norman, OK; 8Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; 9Thermofisher Scientific, San Jose, CA

ThP 387 Metabolic alterations observed in plasma of mice fed high-fat diet; Ioanna Ntai1; Amanda Souza1; Ralf Tautenhahn1; Andreas Huhmer1; 1Thermo Fisher Scientific, San Jose, CA

ThP 388 Annotating and identifying credentialed features in the yeast metabolome; Dhanalakshmi S. Anbukumar1; Michaela Schweiger-Haber1; Miriam Sindelar1; Ethan Stancliffe1; Gary J. Patti1, 2; 1Department of Chemistry, Washington University in St. Louis, St. Louis, MO; 2Department of Medicine, Washington University in St. Louis, St. Louis, MO

ThP 389 Global Metabolic Landscape of Fusobacterium spp in Colorectal Cancer Cells.; Hamzah Hassnein Ahmed1; Iqbal Mahmud, Phd1; Sasanka Sekhar Chukkapalli, Phd1; Ann Progulske-Fox, Phd1; Satya Narayan, Phd1; Timothy J Garrett, Phd1; 1University 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 Peng1; Mei Sun1; Zhibo Yang1; 1University of Oklahoma, Norman, OK

ThP 391 UNTARGET LIPIDOMICS REVEALS A LIPID BIOMARKER PANEL AND KEY METABOLITES FOR THE DETECTION OF COLON CANCER; Patricia Oliveira Carvalho1; Anna Maria Alves De Piloto Fernandes2; Márcia Cristina Fernandes Messias3; Gustavo Henrique Buen Duarte3; Gabrielle Kristine Doratiotto De Santis3; Andréia de Melo Porcari2; Ana Valéria Colnaghi Simionato3; Carlos Augusto Real Martinez2; 1University of Salerno, Fisciano, Italy; 2Bruker Daltonik GmbH, Bremen, Germany; 3Murdoch University, Perth, Australia

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 Piirtilä1; Curt Pettersson1; Mikael Hedeland1; 1Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden

ThP 393 Cancer Metabolic Rewiring in Host-Microbiota Interface; Iqbal Mahmud1; Timothy J Garrett2; 1University of Florida, Gainesville, FL; 2University of Florida, Gainesville

ThP 394 MicroLC-MS/MS Untargeted Metabolomics Analysis of Common Food Products; Tong Shen1; Jeremiah Wells1; Tong Xie2; Remco Van Soest3; Arpana Vaniya1; Jacob Folz1; Oliver Fiehn1; 1West Coast Metabolomics Center, UC Davis, Davis, CA; 2Jiangsu Key Laboratory of Pediatric Respiratory Disease, Nanjing University of Chinese Medicine, Nanjing, China; 3SCIEX, Redwood Shores, CA

ThP 395 MDM2 Copy Number Aberrations Alter Lipid Metabolism in Liposarcoma Tumors, Impacting Response to Atorvastatin Treatment; Andrew Patt1; Bryce Demore1; Andrew Patterson2; Philip Smith2; James Chen1; Ewy Mathe1; 1The Ohio State University, Columbus, OH; 2The Pennsylvania State University, University Park, PA

ThP 396 Differential metabolic responses of Saccharomyces cerevisiae in response to oxidants.; Prajita Pandey1; Amit C. Gujar2; Vladimir Shulavev1; 1University of North Texas, Denton, TX; 2Thermo Fisher Scientific, Austin, Texas
Peptides: Sequence Analysis

ThP 398 | Detection, Evaluation and Validation of single amino acid variants in a PANC-1 Cell Line; Zhijing Tan¹; Jianhui Zhu²; Paul M. Stemmer³; Liangliang Sun⁴; Zhichang Yang⁴; Matthew J. Gaffrey⁴; Kendall Schultz⁴; Anthony J. Cesnik⁵; Xinpei Yi⁶; Michael R. Shortreed⁷; Tujin Shi⁸; David M. Lubman⁹; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor; ³Wayne State University, Detroit, MI; ⁴Michigan State University, East Lansing, MI; ⁵PNPL, Richmond, VA; ⁶Stanford University, Stanford, CA; ⁷Baylor College of Medicine, Houston, TX; ⁸University of Wisconsin, Madison, WI

ThP 399 | EXO vivodegradation of bioactive peptides in equine plasma studied by HILIC-HRMS; Fuyu Guan¹, ²; Savannah Fay¹, ²; Xiaoqing Li¹, ²; Youwen You¹, ²; Mary A Robinson¹, ²; ¹University of Pennsylvania, Kennett Square, PA; ²PA Equine Toxicology and Research Laboratory, West Chester, PA

ThP 400 | Analytical Artifacts and Mitigation Strategies for Sequence Variance Analysis by Peptide Mapping; Stone D.-H. Shi¹; Neelam Khanal¹; Andrew Dykstra¹; Christopher S Spahr¹; Zhongqi Zhang¹; ¹Amgen, Thousand Oaks, CA

ThP 401 | A General Strategy to Improve de Novo Peptide Sequencing based on Deep Learning; Shaokai Wang¹; Bin Ma¹; ¹University of Waterloo, Waterloo, ON

ThP 402 | Force degraded product identification of Liraglutide drug by Mass Spectrometer; Shadab Ahmad¹; Sharwan Kumar¹; Dipankar Malakar¹; Manoj Pillai¹; ¹Scix, Gurugram, India

ThP 403 | Differentiating isomeric amino acid residues in peptides with charge transfer dissociation mass spectrometry (CTD-MS); Halle M. Edwards¹; Praneeth M. Mendi¹; Zachary J. Sasienei¹; Hoi-Ting Wu²; Ryan R. Julian³; Glen P. Jackson¹, ²; ¹C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; ²Department of Chemistry, University of California, Riverside, Riverside, CA; ³Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV

ThP 404 | Identification of Therapeutic Peptides and of its Impurities; Ashish Pargaonkar¹; Laxmi Reddy²; Venkat Reddy²; Srinivasulu Polysetty²; Saurabh Nagpal²; Chidella Kartheek Srinivas²; Saikat Banerjee²; ¹Agilent Technologies India Pvt Ltd, Bengaluru, India; ²Agilent Technologies India Pvt Ltd, Manesar, India; ³Agilent Technologies, BENGALURU, India; ⁴Agilent Technologies India Pvt Ltd, Hyderabad, India

ThP 405 | Exploring the diversity of cysteine-rich natural product peptides via MS/MS fingerprint ions; Nicole C. Parsley¹; Owen L. Williams¹; Leslie M. Hicks¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC

Peptidomics

ThP 406 | Native Peptidomics- An HPLC-MS/MS Approach for Analysis of Tumors' Signature; Stefan Wolfsberger¹; Tanja Panić-Janković²; Sonja Seyfert²; Umesh Kalathiya³; Javier Alfaro³; Ted Hupp⁴; Goran Mitulovic⁵; ¹Department of Neurosurgery at the Medical University of Vienna, Vienna, Austria; ²Medical University of Vienna, KIMCL, Vienna, Austria; ³University of Gdansk, Gdansk, Poland; ⁴University of Edinburgh, Edinburgh, United Kingdom

ThP 407 | DIA MS for Profiling the Neuropeptidomical Changes in Cancer borealis Hemolymph Resulting from Food Intake; Wenxin Wu¹; Kellen DeLaney¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, Wisconsin

ThP 408 | Chromium(III)-Induced Enhanced Protonation Survey of Peptides in Electrospray Ionization; Nnenna E. Dieke¹; Carolyn J. Cassady¹; ¹The University of Alabama, Tuscaloosa, AL

ThP 409 | Neuropeptidomic Study of the Mammalian Subcommisssural Organ (SCO) by High Resolution Mass Spectrometry; Pingli Wei¹; Fengfei Ma²; Woo-Ping Ge³, ⁴, ⁵, ₆; Lingjun Li¹, ²; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³Children’s Research Institute, University of Texas Southwestern Medical Center, Dallas, TX; ⁴Department of Pediatrics, University of Texas Southwestern Medical Center, Dallas, TX; ⁵Department of Neuroscience, University of Texas Southwestern Medical Center, Dallas, TX; ⁶Department of Neurology and Neurotherapeutics, University of Texas Southwestern Medical Center, Dallas, TX

ThP 410 | Label-free and DilSequenceAnalysisDiobar tag quantitative methods for profiling mouse hypothalamic neuropeptidomic and proteomic changes under different gut microbiota environments; Rui Liu¹; Pingli Wei¹; Caitlin Keller³; Dustin Frost³; Shuying Han¹; Tzu-Wen Cross¹; Federico Rey²; Lingjun Li¹; ¹Nanjing University of Chinese Medicine, Nanjing, China; ²University of Wisconsin-Madison, Madison, WI; ³University of Wisconsin-Madison, Madison, Wisconsin

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ThP 412 Development of an automated MHC-associated peptide enrichment method for immunopeptidomics analysis using AssayMAP large capacity cartridges; Samuel Pollock¹; Shuai Wu²; Jerry Han²; Steve Murphy²; ¹Genentech, Inc., South San Francisco, CA; ²Agilent Technologies, Santa Clara, CA

ThP 413 Development of Method for Quantitation and Localization of Hyperglycemic Hormones Implicated in Crustacean Response to Hypoxia; Nhu Quynh Vu¹; Dustin Frost¹; Amanda Rae Buchberger¹; Hsu-Ching Yen¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, Wisconsin

ThP 414 Profiling, imaging, and functional assessment of neuropeptides in the crustacean cardiac neuromuscular system using DIA-MS; Kellen Delaney¹; Tessa Hellenbrand¹; Lingjun Li¹; ¹University of Wisconsin, Madison, Madison, WI

ThP 415 Profiling TOPs-mediated proteolytic pathways in Arabidopsis thaliana; Anthony A. Iannetta¹; Holden T. Rogers¹; Thulafegar Al-Mohanna¹; George V. Popescu²; Sorina C. Popescu²; Leslie M. Hicks³; ¹UNC Chapel Hill, Chapel Hill, NC; ²Mississippi State University, Starkville, MS

ThP 416 CAtlas: an immunopeptidome atlas of human cancer; Xinpei Yi¹,²; Yuxing Liao¹,²; Kai Li¹,²; Bo Wen¹,²; Bing Zhang¹,²; ¹Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; ²Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX

ThP 417 Characterisation of a putative new metabolic hormone in human plasma; Michelle Ciesl¹; Dylan J Harney¹; Mark Larance¹; ¹Charles 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 Maes¹; Stephen Haines¹; Michael Krawitzky²; Christopher Adams²; Gary Kruppa²; Ancy Thomas²; Stefan Clerens¹,³,⁴; ¹AgResearch, Christchurch, New Zealand; ²Bruker Daltonics, San Jose, CA; ³Biomolecular Interaction Centre (Canterbury University), Christchurch, New Zealand; ⁴Riddet 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 Shrestha¹,²; Ivan Villalobos Solis¹,²; Suresh Poudel²; Clemence Bonnot²; Claire Veneault-Fourrey³; Francis Martin³; Paul Abraham³; Robert Hettich¹,²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory (ORNL), Oak Ridge, TN; ³UMR 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. Kandigian¹; James P. Quinn¹; Bianca A. Trombetta¹; Steven E. Arnold¹; Becky C. Carlyle¹; ¹Massachusetts 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. Luehr¹,²; Morris Young¹,²; Leonard J. Foster¹,²; ¹Michael Smith Laboratories, Vancouver, BC; ²University of British Columbia, Vancouver, BC

ThP 422 Immuno-peptidomics: Utilizing cloud computing to identify more peptides in a fraction of the search time; Amol Prakash¹; Benjamin Orsborn²; ¹Optys Tech Corporation, Shrewsbury, MA; ²Proteomic Und Genomic Sciences, Columbia, 21406

ThP 423 An Improved Peptidomics Workflow Using a Multi-nozzle Electrospray Emitter for Capillary Flows; Bertrand Rochat¹,²; Jachen Barbilan¹,²; Patrice Wandel¹,²; Manfredo Quadroni¹,²; ¹University of Lausanne, Lausanne, Switzerland; ²Protein Analysis Facility, Lausanne, Switzerland

ThP 424 Discovery of Tumor associated T cell epitopes through targeted searches of mass spectrometry data; Prathyusha Konda¹; Patrick Murphy²; Shashi Gujar¹; ¹Dalhousie University, Halifax, NS; ²PEI 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
Zirconium(IV)-IMAC for phosphopeptide enrichment in mass spectrometry driven phosphoproteomics; Ignacio Arribas Diez1; Ireshen Govender2; Previn Naicker2; Stoyan Stoychev2, 3; Justin Jordan2, 3; Ole N Jensen1; 1University of Southern Denmark, Odense, Denmark; 2Council for scientific and industrial research, Pretoria, South Africa; 3ReSyn 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 Huang1; Xiaoyan Liu2; Danqing Wang1; Yusi Cui1; Xudong Shi1; Jing Dong2; Mingliang Ye2; Lingjun Li1; 1University of Wisconsin-Madison, Madison, WI; 2Key Laboratory of Separation Sciences for Analytical Chemistry, National Chromatographic R&A Center, Dalian Institute 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 Mullis1; Lim Andrew Lee2; Rebekah Woolsey3; David Quilici; Qian Wang1; 1University of South Carolina, Columbia, SC; 2Integrated Micro-Chromatography Systems, Iro, SC; 3Mitch Hitchcock, Ph.D. Nevada Proteomics Center, Reno, NV

ThP 430
Global phosphoproteomic analysis from low sample amounts enabled by effective phosphopeptide enrichment; Fang Liu1; Momoe Zhou2; Kratika Singhal1; Rowan Matney1; Stefan L. Oliver2; Ann M. Arvin2; Ryan D. Leib1; Allis S. Chien1; 1Stanford University Mass Spectrometry, Stanford University, Stanford, CA; 2Departments of Pediatrics and Microbiology & Immunology, Stanford University School of Medicine, Stanford, CA

PLANTS: SYSTEMS, BIOTECHNOLOGY, AND NATURAL PRODUCTS

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An international laboratory comparison of dissolved organic matter composition by high resolution mass spectrometry: Are we getting the same answer?; Jeffrey A. Hawkes1; Juliana D’andril2; Rachel L. Sleighert3; Hongmei Chen1; Patrick G. Hatcher2; Amna Ijaz1; Maryam Khaksari1; Simeon Schum1; Lynn Mazzaoleni1; Rosalie K. Chu1; Nikola Tolic1; William Kew1; Nancy Hess1; Jitao Lü1; Shuzhen Zhang1; Chen He1; Quan Shi1; Ryan H. S. Hutchins1, 2; Diana C. Palacio Lozano1, 2; Remy Gavard1, 2; Hugh E. Jones1, 2; Mary J. Thomas1, 2; Mark P. Barrow1, 2; Helena Osterholz1, 2; Thorsten Dittmar1, 2; Carsten Simon1, 2; Gerd Gleixner1, 2; Stephanie M. Berg1, 2; Christina K. Remucal1, 2; Nikola Radoman1, 2; Nicholas D. Schmitt1, 2; Jeffrey N. Agar1, 2; Phoebe Zito1, 2; David C. Podgorski1, 2; Uppsala University, Uppsala, Sweden; 1Louisiana Universities Marine Consortium, Chauvin, LA; 2Old Dominion University, Norfolk, VA; 3Michigan Technological University, Houghton, MI; 4PNNL, Richland, WA; 5Chinese Academy of Sciences, Beijing, China; 6China University of Petroleum, Beijing, China; 7University of Alberta, Edmonton, AB; 8University of Warwick, Coventry, United Kingdom; 9Carl von Ossietzky University, Oldenburg, Germany; 10Max Planck Institute, Jena, Germany; 11University of Wisconsin, Madison, WI; 12Catalan Institute for Water Research, Girona, Spain; 13University of Orleans, Orleans, New Orleans, LA; 14Leibniz Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany; 15Stockholm University, Stockholm, Sweden; 16Northeastern University, Boston, MA; 17University of New Orleans, New Orleans, LA

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A large GSK3 signaling network is uncovered by a combination of proximity labeling and phosphoproteomics in Arabidopsis; Chuan-Chih Hsu1; Chang-Ho Park1; Tae-Wu Kim1; Jia-Ying Zhu1; Yu-Chun Hsiao1; Shou-Ling Xu1; Zhi-Yong Wang1; 1Carnegie Institution for Science, Stanford, CA; 2Hanyang University, Seoul, South Korea

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Preserved and variable spatial-chemical changes of lipids across leaves in response to wounding; Susan Velickovic1; Rosalie K. Chu1; Corinna Henkel2; Annika Koch2; Nannan Tao2; Joshua N Adkins1; Christopher Anderton1; Jennifer E. Kyle1; Kent Bloodworth1; Lisa M Bramer1; Shannon Connett1; Kristin E. Burnum-Johnson1; 1Oregon State University, Corvallis, OR; 2DOE Office of Science Graduate Student Research (SCGSR), Oak Ridge, TN; 3Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

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Defining Core Leaf and Root Metabolomes for Sorghum Grown in the Midwestern United States; Amy Sheflin1; Daniel P. Schachtman1; Ellen L. Marsh1; Peng Liu1; Hao Wang1; Corey D Broeckling1; Jessica E Prenni1; 1Colorado State University, Fort Collins, CO; 2University of Nebraska-Lincoln, Lincoln, NE; 3Iowa State University, Ames, IA

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Quantitative proteomics reveals details of the susceptibility pathway of Septoria canker mediated by a Populus trichocarpa G-type lectin receptor-kinase; Ryan R. Lenz1, 2; Paul E. Abraham3; Jessy Labbe3; Wellington Muchero3; Robert L. Hettich3; Jared M. Leboldus1; 1Oregon State University, Corvallis, OR; 2DOE Office of Science Graduate Student Research (SCGSR), Oak Ridge, TN; 3Michigan Technological University, Houghton, MI

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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 Krakowiak1; Sophia Baldszysz1; Oskar Musidla1; Robert Nawrot1; 1Adam 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. Almeida1; Domingos F. Neto2; Gabriel R. A. Carneiro3; Andreza R. B. Farias4; Gilberto B. Domont1; Francisco A. P. Campos5; Fabio CS Nogueira1,3; 1Proteomics Unit, Institute of Chemistry, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, Rio de Janeiro, Brazil; 2Department of Agricultural Sciences, Federal University of Ceará, Fortaleza, Brazil; 3Laboratory of Proteomics/LADETEC, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; 4Department 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 Blakeslee1; Rachel Combs1; Pengfei Bai2; Matthew Bernier2; Nick Choi2; Guo-Liang Wang2; 1The Ohio State University, Wooster, OH; 2The Ohio State University, Columbus, OH

**ThP 440** Enhanced characterization of lignin oligomers and phenolic compounds using CID-MSn combined with HCD-MS2; Woo-Young Song1; Tae-Young Kim1; 1Gwangju Institute of Science and Technology, Gwangju, South Korea

**ThP 441** The tomato root exometabolome and iron-limitation induced changes in exudation profiles; Vineeta Rai1; Oliver Baars1; 1North 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 Kawasaki1; Takeshi Sakai2; Yosuke Sumitomo2; Ken Hayakawa2; Kyoko Nogami2; Heishun Zen3; Akinori Inizawa4; Yasushi Hayakawa4; 1IR Free Electron Laser Research Center, Tokyo University of Science, Noda, Japan; 2Laboratory for Electron Beam Research and Application (LEBRA), Nihon University, Funabashi, Japan; 3Institute of Advanced Energy, Kyoto University, Uji, Japan; 4The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Japan

**ThP 443** Optimisation of Polymer Photoligation Reactions Using Laser Photodissociation Action Spectroscopy; David L. Marshall1; Jan Philipp Menzel2; Benjamin I. McKinnon3; Adam J. Trevitt4; Christopher Barner-Kowollik5; Stephen J. Blanksby1; 1Queensland University of Technology, Brisbane, Australia; 2Queensland University of Technology, Brisbane, Australia; 3University of Wollongong, Wollongong, Australia

**ThP 444** Ultraviolet irradiation degradation analysis of polyethylene terephthalate film using matrix assisted laser desorption/ionization mass spectrometry imaging; Takaya Satoh1; Yusuke Sakuda1; Sayaka Nakamura2; Thierry Fouquet3; Hiroaki Satoh4; Yoshihisa Ueda5; Glen Gregory6; 1JEOL Ltd, Akishima, Japan; 2National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; 3JEOL USA, Inc., Peabody, MA

**ThP 445** Differentiation of Macroyclic and Tadpole Isomers Using UPLC-MS/MS and Radical-Induced Fragmentation Chemistry; Jason M O’Neill1; Scott M Grayson2; Chrys Wesdemiotis1; 1The University of Akron, Akron, OH; 2Tulane 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 Nakamura1; Thierry Nicolas Jean Fouquet1; Robert B. Cody2; Takayuki Ohmura3; Ryoji Satoh3; Hiroaki Satoh4; Yasuhide Naito5; 1National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; 2JEOL USA, Inc., Peabody, MA; 3Hamamatsu Photonics K.K., Iwata, Japan; 4The 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 Goda1; Junichi Masuda2; Manami Kobayashi3; Yoshihiro Hayakawa4; 1Shimadzu Corporation, Hadano, Japan; 2Shimadzu corporation, Kyoto, Japan

**ThP 448** Multiplexed Mass Spectrometric Screening of the Cellular Uptake of Polymer Based Drug Delivery Vehicles Using MALDI-MS; Dheeraj K. Agrohia1; Michael Yandrasits1; Matthew Lindell2; Eric Fort3; 13M, St. Paul, MN; 2University of St. Thomas, St. Paul, MN

**ThP 449** Ultraviolet Photo-activation using Synchrotron Radiation for Tandem Mass Spectrometry of Polyisoxolanes; Inès Aloui1; Véronique Legros1; Alexandre Giuliani1; William Buchmann1; 1Université Paris-Saclay, Univ Evy, CNRS, LAMBE, Evry, France; 2Disco 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 Kalstabakken1; Michael Yandrasits1; Matthew Lindell2; Eric Fort3; 13M, St. Paul, MN; 2University of St. Thomas, St. Paul, MN

**ThP 451** Characterizing photoresist films at the nanoscale with mass spectrometry; Michael Eller1; Mingqi Li2; Xisen Hou2; Stanislav Verkhoturov3; Emile Schweikert4; Peter Trefonas2; 1California State University Northridge, Northridge, CA; 2DuPont Electronics and Imaging, Marlborough, MA; 3Texas A&M University, College Station, TX
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**ThP 453** PolymerSoup: A Novel Tool for De Novo Sequencing of Polymer Mixtures; David Doran; Emma Clarke; Graham Keenan; Emma J Carrick; Cole Mathis; Leroy Cronin; 1University of Glasgow, Glasgow, United Kingdom

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**ThP 456** Agnostic Polymer Detection Using Mass Spectrometry for Astrobiological Samples; Luoth Chou; Natalie Grefenstette; Heather Graham; Chris Kempes; Paul Mahaffy; Sarah Stewart Johnson; 1NASA Goddard Space Flight Center, Greenbelt, MD; 2Santa Fe Institute, Santa Fe, NM

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**ThP 458** Use of PASEF for Accelerated Protein Sequence Confirmation and de novo Sequencing with High Data Quality; Stuart Pengelley; Waltraud Evers; Eckhard Belau; Ilker Sen; Wilfred Tang; Alain Beck; Detlev Suckau; 1Bruker Daltonics, Bremen, Germany; 2Protein Metrics Inc., Cupertino, CA; 3IRPF, 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; Jonathan Jones; Catherine Evans; Maurizio Bronzetti; 1Genedata GmbH, Munich, Germany; 2Genedata Ltd, Cambridge, United Kingdom; 3Genedata AG, Basel, Switzerland; 4Genedata Inc, San Francisco, CA

**ThP 460** Intact Protein Multi-Attribute Method (MAM) that Includes the Identification and Quantification of Protein Clipping Events; Lars Vorwerq; Stuart Pengelley; Waltraud Evers; Eckhard Belau; Detlev Suckau; 1Bruker Daltonics, Bremen, Germany

**ThP 461** Rapid and Confident Identification of Expected and Scrambled Disulfide Bonds in Biologics; Severine Clavier; Hélène Le Borgne; Bruno Genet; Sean Mc Carthy; Kerstin Pohl; 1Sanofi, Vitry Sur Seine, France; 2Sciex, Framingham, MA

**ThP 462** Enhancing the characterization of adeno-associated virus (AAV) vectors by improved UPLC and MS methodology; Ximo Zhang; Stephan Koza; Hua Yang; Lindsey Organtini; Henry Shion; Kamran Anwar; Daniel Gailbraith; Ying Qing Yu; Weibin Chen; 1Waters Corporation, Milford, MA; 2Waters Corps, Milford, MA; 3BioReliance, Rockville, MD

**ThP 463** An automated MS data processing workflow for sensitive detection of low-abundance sequence variants in biopharmaceuticals; Aude Tartiire; Jonathan Jones; Catherine Evans; Peter Haberl; Maurizio Bronzetti; 1Genedata Inc, San Francisco, CA; 2Genedata Ltd, Cambridge, United Kingdom; 3Genedata AG, Basel, Switzerland; 4Genedata GmbH, Munich, Germany

**ThP 464** Characterization of Disulfide Bonds in Bevacizumab Biosimilar Using A Q-TOF Mass Spectrometer; Yonghai Lu; Jie Xing; Zhaqoi Zhan; 1Shimadzu (Asia Pacific) PTE LTD, Singapore, Singapore; 2Shimadzu (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; Florian Fussl; Itzcoatl Gomez Aquino; Joscani Jimenez Del Val; Jonathan Bones; Silvia Millan Martin; 1National Institute for Bioprocessing Research and Training (NIBRT), blackrock, Ireland; 2University 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; Dominique Garceau; Tristan Canò; Caitlin Jaeger; Roy Hegedus; William Hermans; Norman Garceau; Christopher M. Colangelo; 1Agilent, Lexington, MA; 2LakePharma, Worcester, MA

**ThP 467** Intact Mass Analysis using Automated Time-resolved Deconvolution: In-depth Characterization of IgG-type Monoclonal Antibody Subunits; Kate Liu; David Bush; Jonathan Jones; Catherine Evans; Maurizio Bronzetti; 1Genedata Inc, San Francisco, CA; 2Genedata, Lexington, MA; 3Genedata Ltd, Cambridge, United Kingdom; 4Genedata AG, Basel, Switzerland
Improving the analysis of adeno-associated virus (AAV) capsid proteins by a LC-FLR/MS approach for AAV-based gene therapy development; Xiaoying Jin; Ximo Zhang; Zichuan Zhang; Lin Liu; Qiuyu Wang; Yunfan Gao; Joanne Cotton; Stephan Koza; Ying Qing Yu; Weibin Chen; Marc Verhagen; Karen Lee; Claire Davies; Sanofi, Framingham, MA; Waters Corporation, Milford, MA

Biotherapeutic Characterization in Fifteen Minutes: Structures for Lossless Ion Manipulations (SLIM) Ion Mobility for Critical Quality Attribute Identification and Monitoring; James R. Arndt; Kelly L. Wormwood Moser; Liulin Deng; Anisha Yadav; Stephen Krufka; Daniel Debord; Laura Maxon; Mobilion Systems, Inc., Chadds Ford, PA

Identification and Quantitative Analysis of Disulfide Scrambling Events for In-Depth Characterization Studies of Therapeutic Proteins; Magdalena Widgren Sandberg; Jakob Bunkenborg; Thomas Kofoed; Kerstin Pohl; Alphalyse A/S, Odense, Denmark; Sciex, Framingham, MA

Impact of media components (Vitamins) supplementation on glycan profile as a critical quality attribute of an in-house produced monoclonal Antibody; Rohan Shah; Saurabh Nagpal; Anurag S Rathore; Department of Chemical Engineering, Indian Institute of Technology, Delhi, India; Agilent technologies, Gurgaon, India

Glycosylation Profiling of Rituximab using HILIC-LC-FLD glycan mapping and RP-LC-MS glycopeptide mapping; Hongbin Zhu; Joshua Shipman; Milani Rasangika Wijeweera Patabandige; Jason Rodriguez; Connie Ruzicka; David Keire; U.S. FDA, Saint Louis, MO; FDA, Saint Louis, MO; University of Kansas, Lawrence, KS

Characterization and Differentiation of Bispecific Monoclonal Antibodies by Native Mass Spectrometry; Chen Du; Zachary L VanAernum; Wilson Phung; Guanghui Han; Wendy Sandoval; Vicki W Pycock; The Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; Department of Microchemistry, Proteomics and Lipidomics, Genentech, Inc., South San Francisco, CA; San Jose Mass Spectrometry Center, BGI Americas, San Jose, CA

Characterization of Heavily Glycosylated Therapeutics via Proton Transfer Charge Reduction (PTCR); Fred Zinnel; Hirsh Nanda; Harsha Gunawardena; Thermo Fisher Scientific, Somerset, NJ; JOHNSON AND JOHNSON, Spring House, PA

Understanding the structural basis for Alpha-Synuclein aggregation by Fast Photochemical Oxidation of Proteins; Ravi Kant; Prashant N. Jethva; Saketh Chemuru; Harish Kumar; Eva Illes-Toth; Jing Yan; Michael L. Gross; Washington University, St Louis, MO; Washington University, St. Louis, MO; National Centre for Biological Sciences, Bangalore, India

Fighting Counterfeits for Biopharmaceuticals with Accurate Mass Spectrometry; Kerstin Pohl; Esme Candish; Sciex, Framingham, MA; Sciex, Framingham, MA

Coupling a Microchip-Based Image cIEF Separation via ESI to Multiple Mass Spectrometry Platforms for Intact Antibody Characterization; Mariam S Elnaggar; Christopher Herring; Scott Mack; Maggie A. Ostrowski; Erik Gentalen; Intabio, Inc., Newark, CA

Characterization of Charge Heterogeneity of Monoclonal Antibodies Using Microchip CE coupled with TOF MS; Zuzana Demianova; Fang Wang; Sean McCarthy; J. Scott Mellors; Joshua Guerrette; Kerstin Pohl; Sciex, Brea, CA; Sciex, Framingham, MA; 908 Devices, Inc., Boston, MA

Integrating proton transfer charge reduction, multiple activations and synchronous precursor selection improves middle-down analysis of antibodies and antibody-drug conjugates; Ryan Oates; Kristina Szreic; Christopher Mullen; Romain Huguet; Vlad Zabrouskov; John E.P. Syka; Luca Formenti; University of Oklahoma, Norman, OK; Thermo Fisher Scientific, Cambridge Proteomics Research Group, Cambridge, MA; ThermoFisher Scientific, San Jose, CA

Monitoring Local High Order Structure Change for Stressed Biotherapeutics using Native Digestion Peptide Mapping; Dongdong Wang; BioAnalytix, Cambridge, MA

Characterizing the folding of recombinant therapeutic proteins by H/D exchange, native mass spectrometry and ion mobility spectrometry; Nina Kristenko; Eric Largy; Jérôme Haustant; Frédéric Rosu; Cédric Mesmin; Valérie Gabelica; European Institute of Chemistry and Biology, Pessac, France; Merck Biodevelopment SAS, Martillac, France
Development of a Multivariate Model to Assess the Progression of ALS using a Peptide Signature: Allyson L. Mellinger1; Emily H. Griffith2; Michael S. Bererman1, 3; 1Department of Chemistry, North Carolina State University, Raleigh, North Carolina; 2Department of Statistics, North Carolina State University, Raleigh, North Carolina; 3Department of Biological Sciences, North Carolina State University, Raleigh, North Carolina

Quantitative Proteomics Profiling of Formalin-Fixed Paraffin-Embedded (FFPE) Human Colon Pinch Biopsy for Translational Research: Chenhu Hu1; Liang Jin1; John Maul1; Stephanie Gaudette1; Annette Schwartz Sternal1; Yu Tian1; AbbVie, Worcester, MA

Proteomics Characterization of brain extracellular vesicles in the progression of Alzheimer’s Disease: Xavier Gallart-Palau1, 2, Elisabet Vilella1; Aida Serra1; 1PecProteomics, IMDEA Food Research Institute, Madrid, Spain; 2ILSPV, Hospital Universitari Institut Pera Mata, Reus, Spain; 3ILSPV, Hospital Universitari Institut Pere Mata, CIBERSAM, Reus, Spain

High Throughput Protein Quantification for Clinical Research with a New NanoLC System Coupled to a Triple Quadrupole Mass Spectrometer: Linfeng Wu1; Nicolai Bache2; 1Agilent Technologies, Santa Clara, CA; 2Evosep Biosystems, Odense, Denmark

Methionine Oxidation for Improved Multiple Reaction Monitoring (MRM) of the monoclonal antibody Bevacizumab: Vanessa Pinatto Gaspar1, 2; Sahar Ibrahim1, 2; Vincent R. Richard1; Constance A. Sobsey1, 2; René Zahedi1; Christophe H. Borchers1, 2, 4; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 3Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia

Quantitative proteomics analysis of distant metastatic breast cancer using formalin-fixed paraffin-embedded (FFPE) tissues: Dongyoon Shin1; Joonho Park2; Dohyun Han3; Jihye Moon4; Hansuk Ryu4; Youngsoo Kim1; 1Department of Biomedical Sciences, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea; 2Department of Biomedical Engineering, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea; 3Biomedical Research Institute, Seoul National University Hospital, 101 Daehak-ro Chongno-ku, South Korea; 4Department of Pathology, Seoul National University College of Medicine, 103 Daehak-ro Chongno-ku, South Korea

Development of Multiple Reaction Monitoring (MRM) Methods for Therapeutic Drug Monitoring of Monoclonal Antibodies: Vanessa Pinatto Gaspar1, 2; Sahar Ibrahim1, 2; Constance A. Sobsey1, 2; Vincent R. Richard1; Shaun Eintracht1; René Zahedi1; Christophe H. Borchers1, 2, 4; 1Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 2Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 3Department of Diagnostic Medicine, Jewish General Hospital, Montreal, Canada, Montreal, QC; 4Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia

Proteomic analysis of low abundance IgA1-immune complexes in the serum of IgA Nephropathy patients: Mary A. Bunten1; Amanda Proper1; Audra A. Hargett1; Stacy Hall1; Bruce A. Julian1; Jan Novak1; Matthew B. Renfrow1; 1University of Alabama at Birmingham, Birmingham, AL

Characterization of single-shot plasma proteomics performance using the PASEF method and systematic investigation into the quantitative proteome depth: Stephanie Kaspar-Schoenefeld1; Thomas Kosinski1; Romano Hebeler1; Verena Tellstroem1; Markus Lubeck1; Henning Meyer1; Peter Brechlin1; Kristina Marx1; Pierre-Olivier Schmit2; Scarlet Koch1; Matt Willetts3; Dirk Wunderlich1; Nagariuna Nagara1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker Daltonique S.A., Wissenbourg, France; 3Bruker Scientific LLC, Billerica, MA

Deep Serum Proteomics – Impact on sample processing and library approaches on the quantifiable proteome: Raphael Heilig1; Georgina Berridge1; Philip Charles1; Roman Fischer1; 1University of Oxford, UK, Oxford, United Kingdom

Exploring in depth brain proteome of Alzheimer’s disease (AD) with MALDI Imaging Mass Spectrometry in combination with shotgun proteomics: Yumiko Toyama1; Hongsun Park2; Ryo Kajita3; Nobuto Kakuda1; Tomohiro Miyasaka1; Takashi Nirasawa1; Shigeo Murayama1; Nobuyuki Nukina1; Yasuo Ihara2; Yumiko Toyama1; 1Doshisha University, Kyotanabe, Japan; 2Graduate School of Brain Science, Doshisha University, Kyotanabe, Japan; 3Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 4The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Japan

Multiple Reaction Monitoring based targeted proteomics to screen protein biomarkers in Brain tumors: Saicharan Ghantasala1; Nikita Gahoi1; Shuvolina Mukherjee2; Sanjeeva Srivastava1; 1IIT Bombay, Mumbai, India

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A high-throughput platform for proteome and phospho-proteome profiling of matching tumor and adjacent normal tissue samples from thousands of patients; Jakob Vowinckel1; Karel Novy1; Thomas Corwin2; Tobias Treiber1; Vito Dzio1; Roland Bruderer1; Lukas Reiter1; Eike-Cristin von Leitner2; Oliver Rinner1; Claudia Escher1; 1Biognosys AG, Schlieren, Switzerland; 2Indivumed GmbH, Hamburg, Germany

Characterization of a SP3 Method for Streamlined Urine Proteomics; Pamela S. Cantrell1; Xuemei Zeng1; Matthew V. Fagerburg2; Yang Liu1; Nathan A. Yates1, 2; 1Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; 2Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA

Molecular dissection of renal amyloidosis with MALDI - Imaging Mass Spectrometry and shotgun proteomics on paraffin embedded biopsy tissue section; Yume Mukasa1; Jean-paul Duong van Huyen2; Marion Rabant3; Ryu Kajita3; Takashi Nirasawa2; Yumiko Toyama1; Megumi Terada1; Patrick Bruneval4; Hatsue Ishibashi-Useda2; Hironobu Naiki5; Masaya Ikegawa1; 1Doshisha University, Kyotanabe, Japan; 2Necker-Enfants malads Hospital, Paris, France; 3Bruker Japan K.K., Yokohama, Japan; 4Georges-Pombidou European Hospital, Anatomy-Pathology, Paris, France; 5National Cerebral and Cardiovascular Center, Suita, Japan; 6Department of Molecular Pathology, Faculty of Medical Sciences, University of Fukui, Fukui, Japan

Affordable automated proteomics and multiomics sample preparation; Richard Lam1; John Wilson2; John Laycock1; 1Tecan SP, Inc., Baldwin Park, California; 2Protifi, LLC, Farmingdale, New York

Multi-omic characterisation reveals proteome specific trans effects in autosomal chromosomes correlating with erosion of X chromosome inactivation; Alejandro J Brenes1; Harunori Yoshikawa1; Dailla Bensaddek2; Bogdan Mirauta3; Daniel Seaton2; Hao Jiang1; Jens L Hukelmann4; Angus I Lamond1; 1University of Dundee, Dundee, United Kingdom; 2King Abdullah University of Science and Technology, Thuwal, Saudi Arabia; 3European Bioinformatics Institute, Cambridge, United Kingdom; 4Inmatics, Tuebingen, Germany

Quantitative, deep proteomics of precision therapeutics in breast cancer; Michael J Emanuele1; Laura E Herring1; Natalie K Barker1; Xianxi Wang1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC

Comprehensive identification of HSP70/HSC70 Chaperone Clients in Human Cells; Seung Woo Ryu1, 2; Rose Stewart1, 2; Chase Pecto1; Nicolette Ender1, 2; Oshadi Wimalarathne1, 2; Ji-Hoon Lee1, 2; Carlos P. Zanini4; Antonio Chaerkady1; Chelsea Boo1; Antonio Digiandomenico2; Sonja Hess1; 1R&D, AstraZeneca, Gaithersburg, MD; 2BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD

Protein Profiling Confirms Inhibition of Protein Synthesis/Translation Initiation during Exposure to Sorafenib, an Inducer of Ferroptotic Cancer Cell Death; Emily G. Werth1, 2; Presha Rajbhandari1; Prashant Kaushik1; Brent R. Stockwell1; Lewis M. Brown1; 1Columbia University, New York, NY; 2Present address: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT

Label-free Quantitative Serum Proteomics Reveals Mechanistic Insights into Susceptibility to Infection after Thermal Injury; Abby Chiang1; Ajitha Thanabalasuriar2; Margarita Camara2; Ashley Keller1; Raghothama Chaerkady1; Chelsea Boo1; Antonio Digiandomenico2; Sonja Hess1; 1R&D, AstraZeneca, Gaithersburg, MD; 2BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD

Space Travel, Radiation and Human Health: Proteins Secreted by Vasculature under Low Dose Galactic Cosmic Ray Simulation; Jayanta Chakraborty1; Hazeem L. Okunola2; Shahar Goeta1; Emily G. Werth1, 3; Lewis M. Brown1; Peter W. Grabham2; 1Columbia University, New York, NY; 2Columbia University Irving Medical Center, New York, NY; 3Present address: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT

Investigation of hypoxia and calcineurin inhibition-induced global phosphoproteome changes in human RAMOS B cells; Shichen Shen1; Shannon P. Hilchey2; Sailee Rasam1; Mutka G. Palshikar1; Jason Emo2; Juilee Thakar2; Martin Zand2; Jun Qu1; 1University at Buffalo, Buffalo, NY; 2University of Rochester, Rochester, NY

Mouse Quantitative Proteomics Knowledgebase: assays and protein abundance reference ranges in 20 tissues and 3 mouse strains using MRM; Yassene Mohammed1; 2Pallab Bhowmick1; Sarah A. Michaud1; Helena Pérotssova1; David R Goodlett3, 4; Christoph H. Borchers3, 5, 6, 7; 1University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC; 2Leiden University Medical Center, Leiden, Netherlands; 3University of Maryland, Baltimore, Baltimore, MD; 4University of Gdansk, International Centre for Cancer Vaccine Science, Gdansk, Poland; 5Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; 6Proteomics Centre, Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, Quebec; 7Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, Quebec
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ThP 512 | **SLIM-labeling: principles, data processing workflows and applications in quantitative proteomics**; Nicolas Seneca1; Gelio Alves2; Hendrik Weisser3; Laurent Ligniere4; Samuel Terrier5; Lilian Yang-Crosson5; Pierre Poulain5; Gaelle Lelandais5; Yi-Kuo Yu6; Jean-Michel Camadro5; 1Institut Jacques Monod CNRS, Paris, France; 2NIH, Bethesda, Maryland; 3Storm Therapeutics, Cambridge, United Kingdom; 4Institut 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 Magagnotti1; Maria Lombardi2; Chiara Foglieni1; Annapaola Andolfi1; Paolo G. Camici1, 3; 1OSR, Milan, Italy; 2OSR, Milan, Italy; 3Vita-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 Rao1; Timothy Hank1; Jeffrey Savas1; 1Northwestern University, Chicago, IL

ThP 515 | **TWEAK/Fn14 Signaling Induces Synaptic Phosphoprotein Changes in Mouse Brain**; Rong-Fang Gu1; David Nagy1; Benbo Gao1; Christopher Hinckley1; Linda Burkly1; Ru Wei1; 1Biogen, Cambridge, MA

ThP 516 | **Comparison of MS2 and Real-Time Search MS3 Analyses for Lung Proteomes of Hydrogen Sulfide Treated Swine**; Qin Fu1; Zhen Liu2; Ruchika Bhawal1; Elizabeth Anderson1; Robert Sherwood1; Xiangfang Tang1; Hongtu Zhang2; Sheng Zhang2; 1Cornell University, Ithaca, NY; 2Chinese Academy of Agricultural Sciences, Beijing, China

ThP 517 | **Proteomic analysis of C. elegans to decipher species specific activation mechanisms associate with the pharmacological activation of vanilloid receptors**; Jennifer Ben Salem1; Bruno Nkambeu2; Dina N Arvanitis2; Francis Beaudry1; 1Université de Montréal, St-Hyacinthe, QC; 2Université de Toulouse, Toulouse, France

ThP 518 | **Development of non-human dynamic range standard for proteomic quantification applications**; Judy Boland1; Amber Henry1; Pegah Jalili1; Kevin Ray1; Jeffrey Turner1; 1Sheffield Hallam University, SHEFFIELD, United Kingdom; 2Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom; 3Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom

ThP 519 | **Novel Regulators in TNF-α Mediated Insulin Resistance Elucidated by Quantitative Proteomic Analysis**; Rodrigo Mohallem1; Uma K Aryal1; 1Purdue 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 Sallem1; Catherine Duckett2; Vikki A Carolan3; Tanya Klymenko4; Malcolm R Clench5; 1Sheffield Hallam University, SHEFFIELD, United Kingdom; 2Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom; 3Sheffield Hallam University, SHEFFIELD, United Kingdom; 4Sheffield Hallam University, Centre for Mass Spectrometry Imaging, Sheffield, United Kingdom

ThP 521 | **Proteome responses to intermittent fasting across multiple adipose tissue depots**; Dylan J Harney1; Michelle Cielesh1; Kieren Young1; Mark Larance1; 1University of Sydney, Camperdown, Australia

ThP 522 | **Protein changes across lactation in a lowland gorilla and a Bornean orangutan**; Timothy Cleland1; Michael L Power1; 1Smithsonian Museum Conservation Institute, Suitland, MD; 2Smithsonian 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 Ma1, 2; Shichen Shen1, 3; Shihuan Huo1; Ming Zhang1, 3; Yang Qu2; Xiaoyu Zhu1; Chao Xue1; Anthony Vu1; Xinxin Yang1; Shuo Qian1, 2; Qinqing Shen1; Jun Qu1, 3; 1University at Buffalo, Buffalo, NY; 2Roswell Park Comprehensive Cancer Institute, Buffalo, NY; 3New 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 Egbeijogu1; Remilekun O. Lawal1; Luke Richardson2; Fabrizio Donnarumma1; Touradj Solouki1; Kermit K. Murray1; 1Smithsonian Museum Conservation Institute, Suitland, MD; 2Smithsonian Conservation Biology Institute, Washington, DC

ThP 525 | **Proteomics analysis of Neural Crest cells in a developing Xenopus embryo**; Leena Pad1; Jae Ho Yoon2; Dr. Ira Daar2; Dr. Peter Nemes1; 1Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; 2Cancer & Developmental Biology Laboratory, National Cancer Institute, NIH, Frederick, MD

ThP 526 | **Spatially-resolved, 3D-printed Micro-sampling Coupled to Sensitive Nano-LC-MS to accurately image the protein distributions in tissues**; Ming Zhang1; Min Ma1; Shihuan Huo1; Jun Qu1; 1SUNY at Buffalo, Buffalo, NY

ThP 527 | **in depth Proteomics of Hair Follicles of whiskers from W mutant mice clarifies KIT restriction on hematopoiesis and melanogenesis**; Mayuka Kosugi1; Kazuo Kinoshita2; Takashi Nirasawa3; Ryo Kajita3; Nobuto Kakuda4; Masaya Ikegawa4; 1Doshisha University, Kyotanabe City, Kyoto, Japan; 2Shiga Medical Center Research Institute, Moriyama, Japan; 3Bruker Japan K.K., Yokohama, Japan; 4Doshisha University, Kyotanabe, Japan

ThP 528 | **Streamlined sample processing coupled to PASEF strategy for in-depth proteome quantification**; Fabian Hosp1; Katrin Hartinger1; Sebastian Johansson1; Nils A. Kulak1; Sophia Doll1; Lisa Schweizer2; Matthias Mann2; Nagarjuna Nagaraj2; 1PreOomics GmbH, München, Germany; 2OmicEra Diagnostics GmbH, Planegg/Martinsried, Germany; 3Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; 4Bruker Daltonic GmbH, Bremen, Germany
**THURSDAY POSTERS (ThP) Pages 125-164** | All posters will be on-demand content in the mobile app and online planner. Short abstract, Poster PDF, and optional presentation video will be included.

ThP 530
High throughput, spatially-resolved proteomic analysis of a human brain tumour; Simon Davis1; Connor Scott2; Benedikt Kessler3; Olaf Ansorge4; Roman Fischer5; 1Target Discovery Institute, University of Oxford, Oxford, United Kingdom; 2Nuffield 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 Zaman1; Vien Nguyen1; Katalin Prokai-Tatrai1; Laszlo Prokai1; 1University 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 Sharman1, 2; Nathan Heath Patterson1, 2; Danielle B Gutierrez3, 4; Elizabeth K Neumann1, 3; Emma R Guiberson1, 3, 4; Andy Weiss5; William J. Perry1, 4; Daniel J Ryan1, 4; Raf Van de Plas6; Eric P Skara3; Richard M Caprioli1, 3, 4, 5, 6, 7, 8; Jeffrey M Spraggins1, 3, 4, 9; 1Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 2Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Chemistry, Vanderbilt University, Nashville, TN; 5Department of Pathology Microbiology and Immunology, Vanderbilt University, Nashville, TN; 6Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; 7Department of Medicine, Vanderbilt University, Nashville, TN; 8Department 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 Salem1, 2; Marc Kemorgant3; Jason Iacovoni2; Lionel Dahan2; Denis Calise2; Anne Pawy La-Troani4; Francis Beaudy4; Dina N Arvanitis5; 1Universite de Toulouse, Toulouse, France; 2Université de Toulouse, Toulouse, France

ThP 535
An Optimized Sample Preparation Method of Formalin-Fixed Paraffin-Embedded Tissues for Mass Spec Applications; Kara Zehr1; Bhavin Patel2; Amareet Flora2; Jensen Penny2; Sergei Snovida2; Ryan Bomgarder3; 1University of Illinois at Urbana-Champaign, Urbana, IL; 2Thermo Fisher Scientific, Rockford, IL; 3ThermoFisher Scientific, Rockford, IL

ThP 536
Mitochondrial ATP synthase subunit c biogenesis revealed by quantitative MS interactomics; Marek Vrbacky1; Aleksandra Markovic1; Josef Houstek1; Tomas Mracek1; 1Institute 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 Frey1; Zach Rolfs2; Michael R Shortreed3; Yoshihata Kawai4; Lei Lu1; Nathan V Welham5; Lloyd M Smith1; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Department of Surgery, University of Wisconsin-Madison, Madison, WI

ThP 538
Proteogenomics identifies novel biological effects of schizophrenia risk loci; Matthew L Macdonald1; Lora Mcclain1; Lambertus Klei1; Megan Garver1; David Lewis1; Robert Sweet1; Nathan Yates1; Bernie Devlin1; 1University of Pittsburgh, Pittsburgh, PA

ThP 539
Method for comprehensive proteomic analysis of FFPE tissues for potential clinical utilization; Amanda Lorentzian1; Enes Ergin2; Jonathan Bush3; Chinten James Lim2, 4; Gregor S.D Reid2, 4; Christopher A Maxwell2, 4; Philipp Lange2, 3, 4; 1Department of Cell and Developmental Biology, University of British Columbia, Vancouver, British Columbia; 2Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, British Columbia; 3Department of Pediatrics, University of British Columbia, Vancouver, British Columbia; 4Michael 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 Lu1; Lijia Qian1; Wei Liu2; Qiushi Zhang1; Weigang Ge1; Yi Zhu1; Tiannan Guo1; 1Westlake University, Hangzhou, China

ThP 541
First Draft of the In Vivo Beta Cell Proteome by Cell Type Specific Proximity Biotinylation in BirA* Mice; Shiva Ahmadi1; Elham Pourbarkhordariesfandabadi2; Kenichi Kimura3; Anna Egerter4; Martin Breitbach5; Caroline Geissen2; Michael Hesse3; Robert Hardt1; Hubert Schorle3; Bernd K Fleischmann2; Volkmars Gieselmann1; 1Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany; 2Institute for Physiology 1, University of Bonn, Bonn, Germany; 3Institute 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; Hyevoon Kim1, 2; Hophil Min3; Hansuk Ryu1, 4; Dohyun Han2, 4; 1Department of Pathology, Seoul National University College of Medicine, Seoul, South Korea; 2Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; 3Doping Control Center, Korea Institute of Science and Technology (KIST), Seoul, South Korea; 4Seoul National University Hospital, Seoul, South Korea

ThP 543
Comprehensive characterization of the phosphoproteome of gastric cancer from endoscopic biopsy specimens; Jun Adachi1; Yuichi Abe2; Hidekazu Hirano2; Hirokazu Shoji3; Asa Tada1; Junko Isoyama1; Akemi Kakudo2; Daigo Gunji1, 3; Kazufumi Honda2; Narikazu Boku3; Tomonaga Takeshi1; 1National Institutes of...
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<td><strong>Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; 2National Cancer Center Hospital, Tokyo, Japan; 3Kyoto University, Kyoto, Japan; 4National Cancer Center Research Institute, Tokyo, Japan</strong></td>
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### PROTEOMICS: TOP DOWN ANALYSIS II

**ThP 544**

**Improving CZE-MS/MS for both denaturing and native top-down proteomics;** Xiaojing Shen1; Tian Xu1; Liangliang Sun1; 1Michigan 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 McCool1; Liangliang Sun2; Amanda Hummon3; Nicole Beller3; 1Michigan State University, East Lansing; 2Michigan State University, East Lansing, MI; 3The Ohio State University, Columbus, OH

**ThP 546**

**Assessing Regional Heterogeneity of Sarcomeric Proteoforms in Human Hearts by Top-Down Proteomics;** Elizabeth F Bayne1; Stanford Mitchell1; Trisha Tucholski2; Hannah Karp3; Max Wrobbel1; Yang Hu1; Sean McIwain1; Kosake Uijihara1; Joshua Hermesen1; Ying Ge1; 1University of Wisconsin - Madison, Madison, WI; 2University of Wisconsin-Madison, Madison, WI

**ThP 547**

**Capillary isoelectric focusing-tandem mass spectrometry for large-scale qualitative and quantitative top-down proteomics;** Tian Xu1; Xiaojing Shen1; Liangliang Sun1; 1Michigan 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 Kosmopoulou1; Athanasios Smyrnakis1, 2, 3; Dimitris Papanastasiou1; Kyle L. Fort3; Alexander A. Makarov3; Roman Zubarev4; Kyle Brown1; Andrew Alpert2; Song Jin1; Ying Ge1, 3, 4; 1Chemistry Department University of Wisconsin-Madison, Madison, WI 53705; 2PolyLC Inc., Columbia, MD; 3Human Proteomics Program, School of Medicine and Public Health, Madison, WI; 4Department of Cellular and Regenerative Biology-University of Wisconsin-Madison, Madison, WI

**ThP 549**

**Real-time Instrument Control Improves Precursor Selection and Increases Proteoform Identifications in Top-down Mass Spectrometry;** Lei Lu1; Michael R. Shortreed1; Mark Scalf1; Lloyd M Smith1; 1University of Wisconsin-Madison, Madison, WI

**ThP 550**

**A Novel Top-Down Proteomics Method Empowered by Photo-cleavable Surfactant and Hydrophilic Interaction Chromatography for Comprehensive Analysis of Phospholamban Proteoforms;** Austin Carr1; Kyle Brown1; Andrew Alpert2; Song Jin1; Ying Ge1, 3, 4; 1Chemistry Department University of Wisconsin-Madison, Madison, WI; 2PolyLC Inc., Columbia, MD; 3Human Proteomics Program, School of Medicine and Public Health, Madison, WI; 4Department 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 Wang1; Liangliang Sun1; 1Michigan State University, East Lansing, MI

**ThP 552**

**Optimized RAS top-down proteomic assay reveals expanded proteoform landscape in malignant cells;** Kanika Sharma1; Dominic Esposito1; Anna Maciag1; Dwight Nissley1; Frank Mccormick1, 2; Caroline Dehart1; 1NCI RAS Initiative, Cancer Research Technology Program, Frederick National Laboratory for Cancer Research, Frederick, MD; 2Helen 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. Tsybin1; Anton N. Kozhinov1; Natalia Gasilova2; Laure Menin3; Konstantin O. Nagornov1; 1Spectroswiss, Lausanne, Switzerland; 2Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

**ThP 554**

**Proteoform profile of human protamines associated with fertility: a top-down approach;** Marina Gay1; Judit Castillo2; Mar Vilanova1; Ada Soler-Ventura2; Gianluca Arauz-Garofalo1; Laura Villarreal1; Ester Sánchez-Jiménez1; Meritxell Jodar2; Rafael Oliva2; Marta Vilaseca2; 1Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain; 2Institut 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. Butcher1; Ayako Takemori2; Nobuaki Takemori2; Lissa C. Anderson1; 1National High Magnetic Field Laboratory, Tallahassee, FL; 2Proto-Science Center, Ehime University, Matsuyama, Japan

**ThP 556**

**Informatic Solution for the FAIR Storage of Experimentally Verified Proteoforms;** Ryan T Fellers1; Bryan P Early1; Joe B Greer1; Richard D Leduc1; Neil L Kelleher1; Paul M Thomas1; 1Northwestern University, Evanston, IL

**ThP 557**

**Optimization of Quantitative Top-Down Proteomics in Complex Samples using Protein-Level Tandem Mass Tag (TMT) Labeling;** Dahang Yu1; Yanting Guo1; Kellye A Cupp-Sutton1; Zhe Wang1; Mulin Fang1; Xiaowen Liu2; Si Wu1; 1University of Oklahoma, Dept. of Chem & Biochem, Norman, OK; 2Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN

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ThP 558  213 nm Ultraviolet Photodissociation for the Characterization of Diselenide Bridges in Designer Selenocysteine Proteins; Ellie C Watts1; Ross Thyer1; Andrew Ellington1; Jennifer S. Brodbell1; 1University of Texas at Austin, Austin, TX

ThP 559  Top-Down Nanoproteomics Enables Comprehensive Analysis of Low-Abundance Cardiac Troponin I Proteofrms from Human Serum; David S Roberts1; Timothy N Tiambang1; Kyle A Brown1; Yanlong Zhu2, 3; Bifan Chen1, 4; Zhijie Wu1; Stanford Mitchell3, 5; Tania M Guardado-Alvarez1; Song Jin1; Ying Ge1, 2, 3; 1University of Wisconsin-Madison, Madison, WI; 2Human Proteomics Program, School of Medicine and Public Health, Madison, WI; 3Department of Cell and Regenerative Biology, University of Wisconsin, Madison, WI; 4Genentech Inc., South San Francisco, CA; 5Molecular and Cellular Pharmacology Training Program, Madison, WI

ThP 560  Quantitative top-down proteomics identifies novel histone H2A-variant specific C-terminal proteolysis events; Matthew Holt1; Tao Wang2; Nicolas L. Young3; 1Baylor College of Medicine, Houston, TX; 2Baylor College of Medicine, Houston

ThP 561  Selective N-terminal mass defect labelling of proteins for improved de novo top-down sequencing; Lavrentis DIMITRIOS Galanopoulos1; Sam Hughes1; Faye Cruickshank1; Colin Logan Mackay1; David Clarke1; 1University 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 Yang1; Xianmiao Zhang1; Cuihan Ren1; Xiaoan Tang1; John (zhongping) Lin1; Luca C Matassa1; Mike (qingtao) Huang2; Sudhakar Pai2; 1Frontage Laboratories, Inc, Exton, PA; 2Akros 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 Zhang1; Sheng Wang1; Jing Huang1; Xiaoying Jin1; Dawei Zhou1; 1Lab Testing Division of WuXi AppTec, Inc., Suzhou Site, Suzhou, China; 2WuXi AppTec, Cranbury, NJ

ThP 564  Extractable 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; Je Xie1; Wei Zeng1, 2; You Jiang1; Shiying Chu1; Guoqing Shi1; Xinhua Dai1, 2; Xiang Fang1, 2; 1Mass Spectrometry Engineering Technology Research Center, Center for Advanced Measurement Science, National Institute of Metrology, Beijing, People's Republic of China, Beijing, China; 2School 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 Wu1; Saba Harini1; Tyrally Ordinario1; Feng Qin1; Cheng-Yuan Cai2; 1PerkinElmer Inc., Woodbridge, ON; 2PerkinElmer 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 Wang1; Deping Cheng1; 1Alliance 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-Rangel1; Phil Koerner1; J Preston1; Laura Snow1; 1Phenomenex, Torrance, CA

ThP 569  Determination of Pirfenidone and Metabolites in Rat Plasma by Coupling On-Line Fractionation with LC-MS/MS; Ming-Luan Chen1; Jeff Plomley1; Milton Furtado1; Anahita Keyhani1; 1Altasciences, Laval, QC

ThP 570  Rapid, Affordable and Efficient Screening of Blood in People Exposed to Air Pollution; Raminta Zmuidnaite1; Jonathan Lacey1; Christian Jardine1; Ray Iles1; 1MAP 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 Peng1; Ardeshir Khadang1; 1Axis 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 Rane1; Deepit Bhandarkar1; Anant Lohar1; Bhaumik Trivedi1; Purushottam Sutar1; Ashutosh Shelar1; Navin Devadiga1; Shailesh Damale1; Jitendra Kelkar1; Ajit Datar1; Pratap Rasam1; 1Shimadzu 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 Sun1; Renmeng Liu1; Mingming Wang1; Deping Cheng1; 1Alliance Pharma, Inc., Malvern, PA

ThP 574  High Throughput Anti retroviral Drug Metabolite Quantitation from Small Amounts at Subtherapeutic Levels; Farzin Gharahdaghi1; Craig Sykes2; Hans Dewald1; Jose-Luis Gallegos-Perez2; 1Sciex, Framingham, MA; 2Division of Pharmacotherapy and Experimental Therapeutics, University of North Carolina, Chapel Hill, North Carolina
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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; Sean Mccarthy; Esme Candish; Lei Xiong; SCIEX, Redwood Shores, California 1201; Sciex, Framingham, MA

ThP 577 Investigation of whole blood stability during LC-MS/MS bioanalytical method validation; Philip S. Wong; Anna Akrami; Christopher James; Amgen, Thousand Oaks, CA

ThP 578 Development of a Data Processing Approach to Support Ultra High-Throughput MS Acquisition; Mikael Levi; Davide Vecchietti; Hiroyuki Yasuda; Kazuto Mannen; Toru Shiohama; Mitsuhiro Kanazawa; Tairo Ogura; Shimadzu Corporation, Kyoto, Japan; Reifycs Inc., Tokyo, Japan

ThP 579 Determination of Nitrosamine impurities in Pregabalin drug substance using Triple Quadrupole Liquid Chromatography Mass Spectrometry; Chander Mani; Saikat Banerjee; Agilent Technologies, Haryana, India; 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; Haixia Zhang; Albert Vandenberg; 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; Holly Post; Thomas Leitzinger; Jie Ding; PPD, Inc, Middleton, WI

ThP 582 Overcoming data challenges in automated mass spectrometry-based screening of entire compound libraries; Roger Ford; Lope Florez; Aude Tartiere; Stephan Heyse; Genedata, Lexington, MA; Genedata AG, Basel, Switzerland; Genentech Inc, South San Francisco, CA

ThP 583 The QTOF methodology for targeted quantitative analysis with similar sensitivity to triple quadrupole; Bingfang Yue; Loan T Nguyen; Daniel M Anderson; 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; Trey A. Vinke; Katherine E. Barre; Kristin L. Aillon; Suramya Waidyanatha; Bradley J. Collins; MRIGlobal, Kansas City, MO; 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; Prasanth Joseph; Arun Kumar P; Saikat Banerjee; Samir Vyas; Agilent Technologies, BENGALURU, India; 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; Christopher Cousineau; Fumin Li; PPD, Middleton, WI