Oral Presentations

Monday, June 6
9:10-9:30 AM, Stars 1
Combining Rapid Isomer Separations and Physicochemical Property Predictions for Drug Molecules with Differential Mobility Spectrometry
Chang Liu1; J.C. Yves LeBlanc2; Jeffrey Shields3; Hui Zhang4; John S. Janiszewski5; Christian Ieritano6; Luke Melo7; Evan Shepherson8; Mitch Verbuyst9; Moaraj Hasan10
1SCiEX; 2Pfizer; 3University of Waterloo

Tuesday, June 7
8:50-9:10 AM, Hemisfair 3
Second Order Space and Velocity Focusing Time of Flight Mass Spectrometry Using an Accelerator Field Free Region
Robert E. Haufler1; Bill Loyd
SCIEx

Tuesday, June 7
2:50-3:10 PM, Stars 1
Universal LBA/LCMS Workflow for Protein Biotherapeutics PK Analysis in Preclinical Assay
Bruce Aungst1; Caroline Becker1; Xun Wang1; Lei Xiong1; Witold Woroniecki1; YiHAN Li1; Suma Ramagiri2; Hua-fen Liu2; Zamas Lam1
1QPS; 2SCIEx

Wednesday, June 8
3:50-4:10 PM, Stars 4
A Novel Top Down Proteomics Pipeline Utilizing Capillary Electrophoresis Separation and Ultraviolet Photodissociation
Jolene K. Diedrich1, 2; Mathieu Lalaville-Adam3; Qian Chu1; Bryan Fonslow1, 3; James J. Moresco1, 2; Alan Saghatelian3; John R. Yates III1, 2
1The Scripps Research Institute; 2The Salk Institute; 3SCIEx

Thursday, June 9
9:30-9:50 AM, Hemisfair 3
Benchmarking SWATH by LFQBench: a Multi-Centered Study Evaluates and Improves Data-Independent-Acquisition-Based Label Free Quantitation Tools
Pedro Navarro1; Joerg Kuharev1; Ludovic Giller2; Oliver M. Bernhardt2; Brendan Maclean5; Stephen Tate4; Chih-Chiang Tsou4; Lucas Reiter4; George Rosenberger2; Yasset Perez-Riverol1; Alexey I. Nesvizhskii1; Ruedi Aebersold1; Stefan Tenzer4
1University Medical Center of the Johannes Gutenberg, Mainz, Rheinland-Pfalz; 2ETH Zurich, Switzerland; 3Biognosys AG, Switzerland; 4University of Washington; 5SCIEx; 6University of Michigan; 7EMBL-EBI, UK

10:10-10:30 AM, Hemisfair 3
Detection and Quantification of Proteins in SWATH-MS Analysis without Using Spectral Libraries
Stephen A. Tate1; Jamie Sherman; Pradeep Narayanaswamy
SCIEx

4:10-4:30 PM, Hemisfair 2
In depth Sphingomyelin and Triacylglycerol Structure Identification Using Electron Impact Excitation of Ions from Organics (EIEIO) and Mass Spectrometry
Takashi Baba1; J. Larry Campbell2; J.C. Yves LeBlanc3; Paul R.S. Baker
SCIEx

Poster Presentations (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

Monday, June 6
#011
An Automated Sample Extraction and Processing Method Combining Ligand Binding and Mass Spectrometry Analysis for Biotherapeutics Quantitation
Ian Moore
SCIEx

#051
High Resolution CESI-MS Analysis of APTS-labeled N-glycans of Biopharmaceutical Interest
Bryan Fonslow1; Marton Szigel1; Andras Guttmann2
1University of Debrecen, Hungary; 2SCIEx
Poster Presentations (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

Monday, June 6 (continued)

#153
Multiplexed Analysis of 215 Pesticides Using Scout-MRM
Romain Carriere1; Blandine Rougemont1; Christelle Margoum1; Mathieu Le Dréau2; David Cox3; J.C. Yves LeBlanc4; Jerome Lemoine1
1Institut des Sciences Analytiques, Université de Lyon, France; 2IRSTEA, France; 3SCIEX

#166
Quantitation and Identification of Legal and Illicit Drugs in Wastewater in the Low ng/L Range Using Large-Volume Injection and LC-MS/MS
Paul Winkler1; Andre Schreiber2; Michael Scherer3
1SCIEX; 2SCIEX Switzerland

#168
Non-Target Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) – Identification of Unknown Environmental Pollutants
André Schreiber1; KC Hyland; Paul Winkler
SCIEX

#302
Scout-MRM; a Method to Acquire Large Numbers of MRM without Predefined Retention Time
Dave Cox1; Blandine Rougemont1; Romain Carriere2; J.C. Yves LeBlanc1; Jerome Lemoine2
1SCIEX; 2Institut des Sciences Analytiques, Université de Lyon, France

#304
An LC-MS Based Method for Monitoring the Activation of Mesotrypsin and a Strategy for Quantitation in Cellular Secretions
Derek Wachtel1; Sushmit Maitra2; Keith Goodman2; Dan Warren2; Lyle Burton1; Marco Kessler1; Sanjeev Forsyth1; Maria Ribadeneira1
1Ironwood Pharmaceuticals; 2SCIEX

#342
Analysis of Synthetic Nucleotides using Accurate Mass and Ion Mobility
Cynthia Sanderson1; Sushmit Maitra; Keith Goodman
SCIEX

#350
Reducing Isobaric Species by Differential Mobility Spectrometry (DMS) for Infusion-Based Lipidomics
Goncalo Vale1; Jeff McDonald1; Paul R.S. Baker2
1UT Southwestern Medical Center; 2SCIEX

#352
Increasing the Resolving Power of Differential Mobility to Supplement (or Eliminate) LC Separation
J.C. Yves LeBlanc1; Chang Liu; J. Larry Campbell; Brad Schneider
SCIEX

#365
Separation of Positional Isomers of PAHSAs Using LC-MS/MS Coupled with Differential Ion Mobility Mass Spectrometry
Shaokun Pang1; Liling Liu2; Xiaorong Liang2; Amos Baruch2; Leo Wang2; Brian Dean1; Yuzhong Deng1
1SCIEX; 2Genentech Inc.

#420
Sphingolipid Profiling Using Robust and Sensitive LC-MS-MS Method
Shachi Saluja1; Dipankar Malaker2; Manoj Pillai2; Avinash Dasgupta23
1Regional Centre for Biotechnology, India; 2SCIEX India; 3Amity University, India

#477
What Are We Eating? Differential Metabolomic Profiles Reveal an Insight into Our Dietary Habits
Paul Clemens1; Baljit Ubhi2
1SCIEX; 2Pharmascience

#662
Application of TOF MS instrument in Bioanalysis – A Case Study
Shaokun Pang1; Weixing Sun1; Adrien Musuku2; Xavier Misonne3
1SCIEX; 2Pharmascience
**Poster Presentations** (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

**Monday, June 6 (continued)**

#675
Determination of Limaprost, an Analogue of PGE1 in Human Plasma by QTRAP® 6500+ and SelexION®+ Technology
Gangyi Liu1, Chao Zhang1, Wenhai Jin1
1Xuhui Center Hospital, China; 2SCIEX China

Tuesday, June 7

#023
Intact Immunoglobulin Gamma Analysis by CESI-MS
Bryan Fonslow1, 2, Olga Friese1, Ying Zhang1, John Yates III1, K. Steven Cook2, Jason Rouse3
1SCIEX; 2The Scripps Research Institute; 3Pfizer

#076
Large-Scale Quantitative Measurements of Rat Brain Hippocampus Membrane Proteome in Prolonged Simulated Microgravity Model by 2D-SWATH® Mass Spectrometry
Peibin Qin1, 2, Yun Wang1, Lihai Guo1, Yongqian Zhang1, Wenhai Jin1, Yulin Deng2
1SCIEX China; 2School of Life Science, Beijing Institute of Technology, China

#079
Understanding the Square-Wave Nature of Q1 Isolation for Data-Independent SWATH® Acquisition
Randy J. Arnold1, Leroi Desouza1, Christie Hunter1, Patrick Pribil1
1SCIEX

#080
Extending the Depth of Coverage in SWATH® Acquisition with Deeper Ion Libraries
Joerg Dojahn1, 2, Nick Morrice2, Christie Hunter3
1SCIEX Germany; 2SCIEX UK; 3SCIEX

#081
The Use of Smaller Q1 Isolation Windows Improves Reproducibility in SWATH® Acquisition Based Protein Quantification Even at Higher Spectral Acquisition Rate
Dipankar Malakar1, Faraz Rashid1, Manoj Pillai1
SCIEX India

#083
Using Scanning SWATH Windows to Improve Both Quantitative and Qualitative Data Over Conventional SWATH and IDA Methodologies
Nic Bloomfield1, Michael Murphy1, Gordana Ivosev1, Stephen Tate1
1SCIEX

#089
Accelerating Data Independent Acquisition with Microflow Chromatography
Christie Hunter1, Nick Morrice2
1SCIEX; 2SCIEX UK

#115
Proteome-Wide Drug Dose-Response of Prostate Cancer Cell Lines Exposed to Androgen Receptor Antagonists by Microflow-LC SWATH MS Analysis
Ludovic Gillet1, Sabine Amon1, Yasuo Uchida1, Nick Morrice2, Christie Hunter2, Ruedi Aebersold1, 4
1ETH Zurich, Switzerland; 2SCIEX UK; 3SCIEX; 4University of Zurich, Switzerland

#131
Emerging Bioanalytical Tool to Characterize Drug and Drug-Products of Biotherapeutics
Jinal Patel1, 2, Mark Cancilla1, Xiang Yu1, Alina Dindyal-Popescu1, Gordon Payne1, Eva Duchoslav1, Suma Ramagiri1
1SCIEX; 2Merck & Co., Inc.

#132
Improved Data-Independent Workflow Strategies for Small Molecule Identification Using a High Resolution Q-TOF Mass Spectrometer
Alina Dindyal-Popescu1, Keith Goodman1, Eva Duchoslav1, Suma Ramagiri1
1SCIEX
Poster Presentations (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

Tuesday, June 7 (continued)

#197
Is Differential Mobility Chemically Driven? Evidence and Simulations for Chemical Effects as Primary Separation Factor in DMS
Walter Wissdorf1; Bradley B. Schneider1; Tom Covey2; James Hager1; Thorsten Benter1
1Bergische Universität Wuppertal, Germany; 2SCIEX

#199
Analysis of Derivatized Glycans using Differential Mobility Spectrometry
Cathy Lane1; J.C. Yves LeBlanc2; J. Larry Campbell2
1SCIEX UK; 2SCIEX

#203
SelexION® DMS-Based Detergent Interference Removal for Shotgun-Lipidomics Analyses
Cyrus Papan1; Julian D. Langer2
1SCIEX Germany; 2Max-Planck-Institute of Biophysics, Germany

#207
Analysis of Free Drug in Antibody-Drug Conjugate by Reversed-Phase HPLC Coupled with Differential Mobility Mass Spectrometry
Chunang (Christine) Gu1; Marie-France Morissette1; Loren Y. Olson2; Shaokun Pang2; Yi Li1; Colin Medley1; David Russell1
1Genentech; 2SCIEX

#208
Optimizing DMS Separations by Comparing Alpha Functions
Brad Schneider1; Erkinjon Nazarov; J.C. Yves LeBlanc2; Frank Londry; Thomas Covey2
1SCIEX

#224
Food Residue Screening Using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) - Multi-Pesticide Identification and Quantitation
KC Hyland1; Paul Winkler; André Schreiber2
1SCIEX

#382
Should We Care About Peptide Co-elution?
Jamie Sherman1; Stephen Tate2
1SCIEX

#395
Improved Detection Efficiency of a High Dynamic Range Pulse Counting Detection System
Bruce Collings1; Marian Dima; Pascal Martin; Stephen Bruce Locke
1SCIEX

#431
NTOF Geometry for QqTOF
Bill Loyd1; Robert E. Hauffler2
1SCIEX

#492
Automation and Remote Visualization of Screening Data
David M. Cox1; Burkhard Schaefer2; John Gibbons1; Victor Lassinskii3
1SCIEX; 2BSSN Software, Germany

#513
Differentiation of Triacylglycerol Regioisomers Using Differential Ion Mobility Spectrometry
Jinyuan Wang1; J. Larry Campbell; Paul R.S. Baker
1SCIEX

#541
Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway
Loren Y. Olson1; Baljit Ubhi
1SCIEX
**Poster Presentations** (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

**Tuesday, June 7 (continued)**

**#710**  
Rootstock Influences Protein Profile at Different Stages of Berry Development in Grape, as Revealed by Whole Proteome Analysis Using HRMS  
Smita Maske1; Anuradha Upadhyay1; Satisha Jogaiah1; Akanksha Singh2; Dipankar Malakar2; Manoj Pillai2; Kaushik Banerjee1  
1ICAR-National Research Centre for Grapes, India; 2SCIEX India

**Wednesday, June 8**

**#059**  
Complete Characterization of Biotherapeutic Proteins by Automated Data Processing on High Resolution Accurate Mass Spectrometry with SWATH® Acquisition  
Milla Neffling*; Yang Shi; Dominic Gostick; Doug Simmons  
SCIEX

**#066**  
Deep Profiling of Extracellular Vesicles in µL-Scale Plasma Samples Using Miniaturized Isolation Combined with Advanced Separation and MS Data Acquisition  
Simion Kreimer1; Arseniy M. Belov1; Rosa I. Viner2; Marcia Santos3; Barry L. Karger1; Alexander R. Ivanov1  
1Northeastern University; 2Thermo Fisher Scientific; 3SCIEX

**#158**  
High Throughput Screening-ADME; Transitioning from Triple Quadrupole to High Resolution Accurate Mass Spectrometry  
Jason Causon1; Graeme Clark2  
1SCIEX UK; 2Cyprotex, UK

**#159**  
Utilizing High Resolution Accurate Mass Spectrometry for Quantification, MRMHRI and SWATH® Acquisition Workflows  
Jason Causon1; Lee Mendi2; Donna-Michelle Smith2; Neil Devenport3; Thomas Knapman1; Milla Neffling1  
1SCIEX UK; 2CRUK Cambridge Institute - University Of Cambridge, UK

**#193**  
Direct Analysis of PFAAs in Water Using Differential Mobility Spectrometry-Mass Spectrometry  
Matthew Noestheden1; KC Hyland1; Simon Roberts1; Chris Higgins1  
1SCIEX; 2Colorado School of Mines

**#266**  
Illegal Drugs Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time- Mass Spectrometry (TDP/DART-MS)  
Hiroko Abe1; Chiakko Takei1; Yasuo Shida1; Motoshi Sakakura1; Teruhisa Shiota1; Kayako Suga3; Daisuke Yajima1; Hirotaro Iwase6  
1University of Chiba, Japan; 2BioChromato, Inc., Japan; 3University of Yamanashi, Japan; 4AMR Inc., Japan; 5SCIEX Japan; 6University of Tokyo, Japan

**#496**  
A Multiwell Magnetic Mixer for Automated Sample Preparation  
Chang Liu; Don W. Arnold; Thomas R. Covey*  
SCIEX

**#533**  
Lipid and fatty acid analysis in grape seeds and grape seed oil with High Resolution Mass Spectrometry  
Zareen Khan1; Akanksha Singh2; Ahammed Shabeer T.P.1; Manoj Pillai1; Kaushik Banerjee1  
1National Referral Laboratory, ICAR-National Research Centre for Grapes, India; 2SCIEX India

**#585**  
A Novel Targeted Metabolic Profiling Workflow for Simultaneous Reverse Phase and HILIC microflow LC-MS/MS Analysis  
Daniel M. Warren*; Jeffrey D. Miller  
SCIEX
**Wednesday, June 8 (continued)**

### #615
**Improving the Sensitivity for an Immunocapture LC-MS Assay of Infliximab in Rat Plasma Using Trap-and-Elute MicroLC-MS**
Remco van Soest*; Lei Xiong
SCIEX

### #628
**Host Cell Protein Analysis by Microflow-LC High Resolution SWATH-MS of Vaccine Samples Under Development**
Søren Heissel*; Milla Neffling1; Rikke Raan Lund2; Marie Grimstrup3; Nick Morrice2; Anne Fich Holmberg3; Max Per Kristiansen3; Ingrid Kromann4; Peter Hejrup5; Ejvind Mørtz5
1Department of Biochemistry and Molecular Biology, University of Southern Denmark, Denmark; 2SCIEX UK; 3Alphalyse A/S, Denmark; 4Statens Serum Institut, Denmark

### #629
**Highly Sensitivity and Reproducible MRM-Based Quantitation of Follicle Stimulating Hormones (FSH) in Human Plasma Using the QTRAP® 6500 System**
Faraz Rashid*1; Rahul Baghla1; Prashant Kale2; Manoj Shukla2; Milin Shah2; Dipankar Malakar1; Anoop Kumar1; Manoj Pillai1
1SCIEX India; 2Lambda Therapeutic Research Ltd, India

### #654
**A New Approach to the Analysis of Intact Major Urinary Proteins (MUPs) from Mouse Urine by CESI-MS**
Stephen J. Lock*1; Robert J. Beynon2; Guadalupe Gomez-Baena2; Edna Betgovargez2
1SCIEX UK; 2Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, UK; 3SCIEX

### #692
**Comprehensive Relative Quantification of the Cytochromes P450 by Micro-LC and SWATH® Acquisition and Data Processing Using Cloud Computing**
Rosalind E. Jenkins1; Sibylle Heidelberger2; Thomas Knapman2; Francesco Brancia2; Neil Kitteringham1; Kevin B. Park1; Mark Cafazzo*3
1MRC Centre for Drug Safety Science, UK; 2SCIEX UK; 3SCIEX

### #028
**Surface Acoustic Wave Nebulization – Mass Spectrometry on a TripleTOF® Mass Spectrometer**
Thomas Schneider1; Benjamin L. Oyler1; J. Larry Campbell2; J.C. Yves LeBlanc2; Tom Covey2; Gloria S. Yen2; Erik Nilsson3; David R. Goodlett1
1University of Maryland School of Pharmacy; 2SCIEX; 3Deurion LLC

### #256
**Scout-MRM: Extended Portability of Large Multiplexed Peptide Assay**
Blandine Rougemont1; Romain Carriere1; Sophie Ayciriex1; Jean Marie Lacroix1; David Cox2; J.C. Yves LeBlanc2; Jérôme Lemoine1
1Institut des Sciences Analytiques, Université de Lyon, France; 2UGSF UMR, France; 3SCIEX

### #330
**Differential Complex Lipid Plasma Profiles Reveal Perturbations in Preeclampsia**
Baljit Ubhi*1; Katherine Williams1; Susan Fischer2
1SCIEX; 2UCSF

### #351
**Research into Lysosomal Storage Metabolism Using Plasma Lipid Characterization by LC-MS/MS**
Sibylle Heidelberger1; Daniel Blake1; Rachel Webster1; Karen Smith2; Martin Rohr3
1SCIEX UK; 2Queen Elizabeth Hospital Birmingham, UK

### #353
**Differential Complex Lipid Plasma Profiles Reveal Perturbations in Preeclampsia**
Baljit Ubhi*1; Katherine Williams1; Susan Fischer2
1SCIEX; 2UCSF

### #370
**Software: Nexus Point of a Targeted Lipid Analyzer**
Pauline J. Vollmerhaus1; Baljit K. Ubhi1; Sarada Tanikella1; Peter Zhu2; Corey D. DeHaven2
1SCIEX; 2Metabolon
Poster Presentations (all posters are located in the Poster/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:30-2:00 PM)

Thursday, June 9 (continued)

#413 Carbonic Anhydrase Inhibitory Potential of Lagenaria siceraria Stand and Identification of Its Bioactive Compounds - An LC-MS/MS Approach
Joydeb Chanda1; Pulok K. Mukherjee1; Rajarshi Biswas1; Dipankar Malakar2; Manoj Pillai2
1School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, India; 2SCIEX India

#439 LC-MRMHR QTOF MS Based Measurement of Metabolite Exchange between Pancreatic Cancer Associated Fibroblasts and Cancer Cells
Li Zhang1; Christopher Hallbrook2; Daniel Kremer2; Shaokun Pang2; Jeff Miller2; Maureen Kachman1; Charles Burant1; Costas Lyssiotis2
1Michigan Regional Comprehensive Metabolomics Resource Center; University of Michigan; 2Department of Molecular and Integrative Physiology, Internal Medicine, Medical School, University of Michigan; 3SCIEX

#440 Quantitation of Nucleotides and Nucleosides without Derivatization Using Transient Isotachophoresis-Capillary Electrophoresis Coupled to Tandem Mass Spectrometry
Jose Luis Gallegos Perez
SCIEX

#473 An Alternative and More Sensitive Approach for the Analysis Ofneuropeptides in Biological Samples
Stephen J. Lock1; Edna Betgoverngez2
1SCIEX UK; 2SCIEX

#552 Biosimilar Insulin Characterization: Top/Middle/Bottoms Up Approaches
Rishitant Gupta1; Milthon Bhatt1; Annu Uppal1; Archana Krishnan1; Sanjay Sonar1
1Bigenomics, India; 2SCIEX India

#564 On-line Disulfide Cleavage for Structural Characterization
J.C. Yves LeBlanc; Tanya Gamble
SCIEX

#626 Improving Speed and Robustness of DIA Quantitation Using Longer microLC Columns
Remco van Soest; Christie Hunter; Gavin Fischer
SCIEX

#629 Quantification of Low-abundant GDF-11 and GDF-8 in Human Serum/Plasma Using LC/MS/MS Analysis after Depleting Bio-Complexity by Cation Ion Exchange SPE
Liming Peng1; Srinivasan Krishnan1; Shalender Bhasin1
1Brigham and Women's Hospital; 2SCIEX

#684 Highly Sensitive LC-MS/MS Method for the Quantification of Fluticasone Propionate in Human Plasma, Feasible for Reinjection and Repeat Analysis
Jeyan Albert1; Praveen V. Kumar2; Manoj Pillai1; Ravi Sekhar K2; Anoo Kumar1
1SCIEX India; 2Lupin Bioresearch Center, India

#696 Quantitation of Pegylated Drug Conjugate Interferon Alfa-2b in Human Serum using the QTRAP® 6500 System
Faraz Rashid1; Dipankar Malakar1; Anoo Kumar1; Manoj Pillai1; Praveen Kumar Vittal1; Manoj Job2; Ravi Sekhar K2
1SCIEX India; 2Lupin Bioresearch Center, India

#698 Highly Sensitive and Selective Bioanalytical Quantitation Method forDocetaxelin Human Plasma
Santosh Kapil Kumar Gorti1; Aman Sharma; Jeyan Albert; Anoo Kumar; Manoj Pillai
SCIEX India