



Welcome to the 62nd ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Baltimore Convention Center. Corporate Member hospitality suites are located in the Hilton Hotel.

SPONSORS

ASMS gratefully acknowledges the support of these companies.



CONFERENCE SPONSORS



CONTRIBUTORS

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Titles in the following sections are provided by authors. The complete abstracts are available online: www.asms.org

The PDF document of proceedings submissions for orals and posters may be viewed online one day after presentation at the conference.

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GENERAL INFORMATION

REGISTRATION is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm on Monday through Thursday.

SUNDAY TUTORIAL SESSION, 5:00 - 6:30 PM

Exhibit Hall AB, level 1



5:00 - 5:45 pm
Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know but Were Afraid to Ask

Lucinda Cohen
Merck Research Laboratories



5:45 - 6:30 pm
Imaging Mass Spectrometry

Ron M.A. Heeren
FOM-AMOLF

SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM

Exhibit Hall AB, level 1



Welcome, Jenny Brodbelt,
University of Texas, Austin
ASMS Vice President for Programs



The James Webb Space Telescope: From First Light to the Search for Earth 2.0

Jason Kalirai
Telescope Science Institute

SUNDAY WELCOME RECEPTION, 7:45 - 9:00 PM

Exhibit Hall C-G. Conference name badge is required.

PLENARY SESSIONS

MONDAY, 4:45 - 5:30 PM

AWARD LECTURE

Exhibit Hall AB, level 1



Award for a Distinguished Contribution in Mass Spectrometry

Richard M. Caprioli
Vanderbilt University

TUESDAY, 4:45 - 5:30 PM

AWARD LECTURE

Exhibit Hall AB, level 1



Biemann Medal

Lingjun Li
University of Wisconsin-Madison

THURSDAY, 4:45 - 5:30 PM

PLENARY LECTURE

Exhibit Hall AB, level 1



How the Genome Folds

Erez Lieberman Aiden
Baylor College of Medicine and
Rice University

DON'T MISS

• ASMS MEETING, WEDNESDAY, 4:45 - 5:30 PM

Ballroom I, level 4

Enjoy a beverage while you applaud awards, hear about new initiatives, and more!

• CLOSING EVENT, THURSDAY, 6:30 - 9:00 PM National Aquarium

Let's celebrate! Enjoy all the aquarium has to offer including an Imax film and a dolphin event. Complete your tour with music provided by a talented group of your colleagues. Ticket is required, \$30.



ORAL SESSIONS are 8:30 - 10:30 am and 2:30 - 4:30 pm on Monday through Thursday.

Session A (MOA, TOA, WOA, ThOA).....Exhibit Hall AB, level 1
 Session B (MOB, TOB, WOB, ThOB).... Room 307-308, level 3
 Session C (MOC, TOC, WOC, ThOC)... Room 309-310, level 3
 Session D (MOD, TOD, WOD, ThOD)... Room 314-317, level 3
 Session E (MOE, TOE, WOE, ThOE)..... Ballroom I, level 4
 Session F (MOF, TOF, WOF, ThOF)..... Ballroom II, level 4
 Session G (MOG, TOG, WOG, ThOG)..... Ballroom III, level 4
 Session H (MOH, TOH, WOH, ThOH)..... Ballroom IV, level 4

ORAL PRESENTATIONS are projected from ASMS computers running Microsoft Office 2010. Speakers are required to use the ASMS computers for their presentations.

SPEAKERS must load presentations at least one day prior to their talks. The speaker room is 330 (behind conference registration area) and is open with a technician according to this schedule:

Sunday: 10:00 am - 8:00 pm
Monday through Wednesday: 7:30 am - 5:00 pm

POSTERS AND EXHIBIT BOOTHS are in Exhibit Hall C-G. The Hall is open:

Sunday Reception7:45 pm - 9:00 pm
 Monday - Wednesday7:30 am - 8:00 pm
 Thursday7:30 am - 3:00 pm

POSTER SET-UP is 7:30 am on the day scheduled and removal is 7:30 - 8:00 pm on the same day. Posters should not be removed early. Thursday posters must be removed by 3:30 pm. **Refer to the poster numbers in this final program for board assignments.** Presenters should supply pushpins or Velcro to mount their posters.

POSTER SESSIONS are 10:30 am - 2:30 pm, Monday through Thursday. Special "themed refreshments" will be offered 1:30 - 2:30 pm daily.

POSTER AUTHORS must be present at posters on scheduled days at these times.

10:30 am - 1:00 pmOdd-numbered posters
 12:00 - 2:30 pm Even-numbered posters

Presenters who must leave a poster unattended should post a return time. Presenters should wear "Poster Presenter" badges which are available at the poster supply counter.

Posters should not be removed before 7:30 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed at 2:30 pm.

LUNCH CONCESSIONS in the Poster/Exhibit Hall offer a variety of options to dine and network while taking a break from posters. Concessions are open 11:00 am - 2:00 pm, Monday through Thursday.

EXHIBITORS must staff exhibit booths as follows:

Sunday Reception7:45 pm - 9:00 pm
 Monday - Thursday10:30 am - 2:30 pm

WORKSHOPS are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function area on level 3.

DINNER BREAK, 7:00 - 8:00 PM is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

SPECIAL PROGRAM FOR UNDERGRADUATE STUDENTS

- **Poster competition**, 7:45 - 9:00 pm, Sunday, Poster/Exhibit Hall
- **Breakfast Tutorial** "Make the Most of ASMS: What to See, Hear and Do!" 7:00 - 8:15 am, Monday, Room 319 (beverages and pastries provided)
- **Meet the Experts** at lunch tables reserved for undergraduate students, 12:00 - 1:00 pm, Monday, Poster/Exhibit Hall

FREE WiFi ACCESS is provided in the Poster/Exhibit Hall. Computers are provided at stations throughout the convention center.

CONFERENCE PROCEEDINGS will be published online. Visit www.asms.org after July 21 to view or download the Proceedings. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker web casting slides will be printed to PDF and used for speakers who fail to submit.**

WEB CASTING includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to www.asms.org, select "web casting" on the annual conference page, and enter your last name and the User ID printed on your conference name badge.

CORPORATE HOSPITALITY SUITES may be open 8:00 - 11 pm, Monday through Wednesday. Suites are located in the **Hilton Hotel**.

CAREER CENTER is located in the Poster/Exhibit Hall. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview booths must be reserved one day in advance.

Sunday7:45 - 9:00 pm
 Monday - Wednesday.....7:30 am - 5:00 pm
 Thursday7:30 am - 2:30 pm

GUEST REGISTRATION (\$10) includes designated name badge and entrance to the Sunday evening reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

CONCIERGE DESK in the conference registration area offers information on transportation, attractions and restaurants.

GENERAL INFORMATION

CORPORATE BREAKFAST SEMINARS are hosted by some Corporate Members. Breakfast seminars are located in the convention center and start at 6:45 am on scheduled day. **Please reserve a seat at company exhibit booths.**

MONDAY	
Company	Convention Center Location
AB SCIEX	Room 343-344
AB SCIEX	Room 345-346
AB SCIEX	Room 347-348
Advanced Chemistry Development (ACD)	Room 328
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
EMD Millipore	Room 336
LECO	Room 327
Shimadzu	Room 337
TUESDAY	
Company	Convention Center Location
AB SCIEX	Room 343-344
AB SCIEX	Room 345-346
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
LECO	Room 327
New Objective	Room 328
Phenomenex	Room 329
Prosolia	Room 336
Shimadzu	Room 337
WEDNESDAY	
Company	Convention Center Location
AB SCIEX	Room 343-344
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
LECO	Room 327
Phenomenex	Room 329
Protea Biosciences	Room 328
Shimadzu	Room 337
Tecan	Room 336
THURSDAY	
Company	Convention Center Location
Shimadzu	Room 337
Thermo Scientific	Room 339-340

MEDIA EVENTS

Corporate media sessions are scheduled on Monday and Tuesday for members of the press and financial institutions.

Company	Monday	Hilton Hotel Location
Bruker Daltonics	8:00-9:00 am	Key Ballroom 6
Shimadzu	9:30-10:30 am	Holiday Ballroom 6
AB SCIEX	11:00 -12:00 pm	Key Ballroom 7
Agilent Technologies	1:30-2:30 pm	Key Ballroom 5
Thermo Scientific	3:00-4:00 pm	Holiday Ballroom 1-3
Waters Corporation	4:30-5:30 pm	Key Ballroom 8
Company	Tuesday	Location
PerkinElmer	9:30-10:30 am	Holiday Ballroom 4-5

CONFERENCE REGULATIONS

- Name badge is required for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- No smoking is permitted in the convention center.
- Cell phones must be turned off in oral sessions.
- No photography or recording is allowed in oral sessions or in the Poster/Exhibit Hall.
- Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without the express written authority of the author of the material presented. Such materials that are published in print or online must contain appropriate credits for all quotations and photographs.
- The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. No signs on easels are permitted.
- Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos on slides or posters may appear only one time in the presentation.

HOTELS AND TRANSPORTATION

CONFERENCE HOTELS

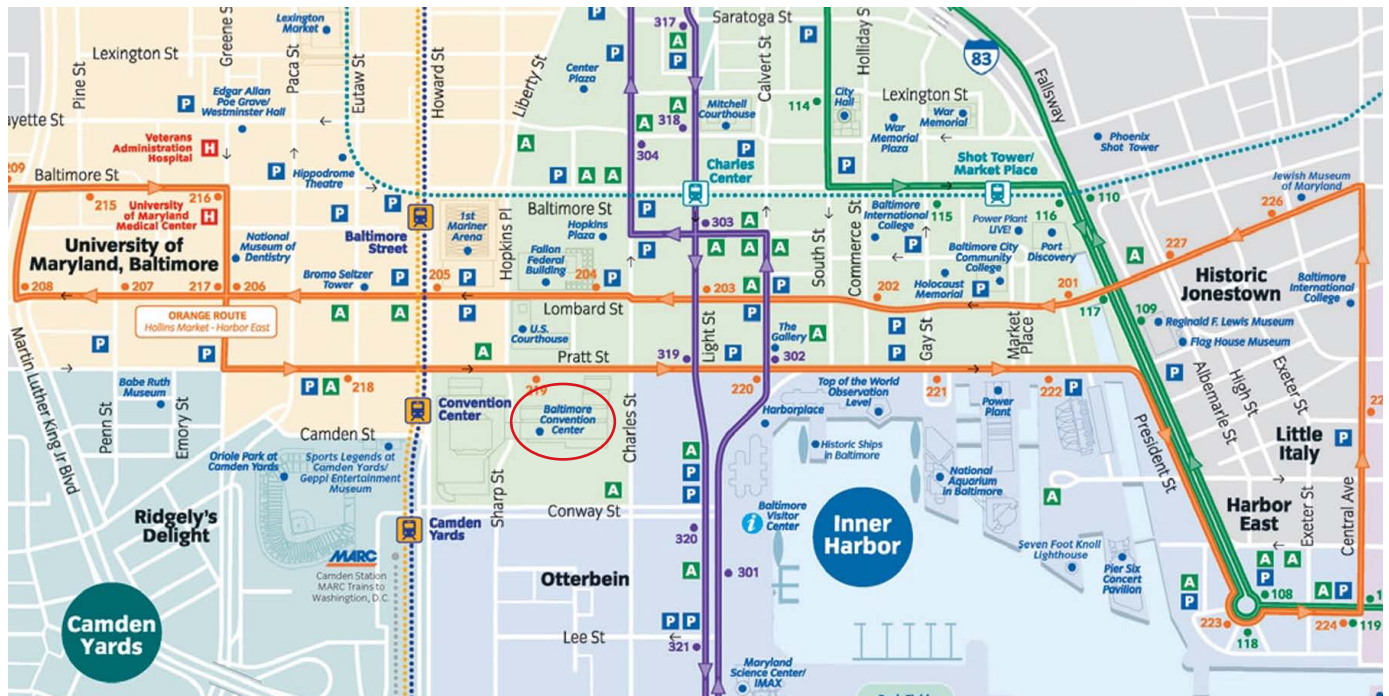
Hotel	Map No.	Telephone
Days Inn Inner Harbor	1	410-576-1000
Hampton Inn	2	410-685-5000
Hilton Baltimore	3	443-573-8700
Holiday Inn Inner Harbor	4	410 685-3500
Hyatt Regency	5	410 528 1234
Lord Baltimore	6	443 977-4092
Marriott Inner Harbor	7	410-962-0202
Monaco Baltimore	8	443-692-6170
Renaissance	9	410-547-1200
Sheraton City Center	10	410-752-1100
Sheraton Inner Harbor	11	410-962-8300

HOTEL MAP



TRANSPORTATION

Travel free throughout the heart of downtown Baltimore on the Charm City Circulator. The orange line connects many attractions and hotels to the Baltimore Convention Center. Image below shows bus stops.





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Congratulations

to these members who were elected to the ASMS Board

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Jennifer Watson
Cindi Lilly, Miquela Sena
Marin Walker, Brent Watson

INTEREST GROUP COORDINATORS

<i>Analytical Laboratory Managers</i>	Brett Phinney
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<i>Biotherapeutics</i>	Li Tao Arindam Roy
<i>Clinical Chemistry</i>	Cory Bystrom Brett Holmquist
<i>Data Independent Acquisition</i>	Yishai Levin
<i>DNA/RNA</i>	Norman Chiu Michael McGinley
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<i>Energy, Petroleum & Biofuels</i>	Patrick Hatcher Lateefah Stanford
<i>Environmental Applications</i>	Kerry Peru Chris Gill
<i>Flavor, Fragrance and Foodstuff</i>	Marc Engel Timothy Croley
<i>Forensics & Homeland Security</i>	Glen Jackson Guido Verbeck
<i>FTMS</i>	Nathan Kaiser Franklin Leach
<i>Fundamentals</i>	George Khairallah Jos Oomens
<i>H/D Exchange, Covalent Labeling & Cross Linking</i>	David Schriemer Joshua Sharp
<i>Imaging MS</i>	Liam McDonnell Zoltan Takats
<i>Ion Mobility MS</i>	Matthew Bush Erin Baker
<i>Ion Trap MS</i>	Daniel E. Austin Yu Xia
<i>Lipids & Lipodomics</i>	Stephen Blanksby
<i>LC/MS Related Topics</i>	Amanda Berg Helene Cardasis
<i>Metabolomics</i>	Gary Patti Sunia Trauger
<i>Metal Ion Coordination Chemistry</i>	Benjamin Bythell Mike Van Stipdonk
<i>Peptide Fragmentation</i>	Sharon Pitteri
<i>Pharmaceuticals</i>	Brian Furmanski Shawna Hengel
<i>Photoionization MS</i>	Jack Syage Ralf Zimmerman
<i>Polymeric Materials</i>	William Erb Gyorgy Vas
<i>Quantitative Intact Proteomics</i>	Edward Dratz

<i>Regulated Bioanalysis</i>	Fabio Garofolo
<i>Undergraduate Research in MS</i>	J.C. Poutsma Elaine Marzluff
<i>Young Mass Spectrometrists</i>	Olga Friese Dian Su

COMMITTEES

<i>Asilomar Conference (ACMS)</i>	Ryan Julian, Chair Glen Jackson Sharon Pitteri Scott McLuckey
<i>Corporate Liaison</i>	Gary Valaskovic, Chair Scott McLuckey Karen Anspach, Phenomenex Carla Marshall-Waggett, New Objective Bez Moghadam, Thermo Scientific Lance Nicolaysen, Waters Qihui Ni, EMD Millipore Johnny Cardenas, AB SCIEX
<i>Digital Communications</i>	Michael MacCoss, Chair Bin Ma Nathan Yates
<i>Education</i>	Gavin Reid, Chair Erin Carlson Michael Fitzgerald Elaine Marzluff Darrin Smith
<i>Nominating</i>	Barbara Larsen, Chair Hilkka Kenttamaa Joseph Loo Christine Miller Nathan Yates
<i>Publications</i>	David Muddiman, Chair Michelle Cilia Jessica Prenni Brandon Ruotolo Yu Xia Michael Gross (<i>ex officio</i>)
<i>Sanibel Conference</i>	Jon Williams, Chair Neil Kelleher Erin Baker J.C. Poutsma

ARCHIVIST

Michael Grayson

AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2014 RECIPIENT: RICHARD M. CAPRIOLI

Award Lecture: 4:45 pm, Monday, Exhibit Hall AB, level 1



Dr. Richard M. Caprioli is awarded the 2014 ASMS Award for a Distinguished Contribution in Mass Spectrometry for the development of MALDI Imaging Mass Spectrometry and its application to molecular mapping of tissues in biology and medicine.

Professor Caprioli's work led to a new paradigm for molecular imaging of tissues, founded on the development of matrix assisted laser desorption ionization (MALDI) imaging mass spectrometry. This is now a burgeoning application of mass spectrometry whereby molecular measurements can be made directly from tissues, adding significantly to the information that can be obtained from these specimens.

This work has made significant contributions to the study of proteins, lipids, metabolites, and pharmaceutical compounds. Since publication of Professor Caprioli's seminal 1997 paper (Anal. Chem. 69(23), 4751-4760) showing the power of MALDI imaging mass spectrometry for tissue analysis, he has pioneered advancements in sample preparation, instrumentation, and informatics approaches that have considerably advanced the technology and made it accessible to hundreds of laboratories worldwide.

The impact of his work is evident in the numerous commercial platforms that employ this technology. Approximately 2,500 papers have been published to date on the subject of MALDI imaging mass spectrometry.

Dr. Caprioli is the Stanford Moore Chair in Biochemistry and Director of the Mass Spectrometry Research Center at Vanderbilt University. Scientist in the Biological Sciences Division and Director of Proteomics Research at Pacific Northwest National Laboratory (PNNL).

BIEMANN MEDAL

2014 RECIPIENT: LINGJUN LI

Award Lecture: 4:45 pm, Tuesday, Exhibit Hall AB, level 1



Dr. Lingjun Li is awarded the 2014 Biemann Medal for the number and depth of her contributions in the field of mass spectrometric study of neuropeptides and functional peptidomics.

Professor Lingjun Li's research program is focused on the development of novel and improved mass spectrometry (MS)-based tools in conjunction with microseparation techniques to study challenging neuroscience problems including functional discovery of neuropeptides and biomarker discovery in neurodegenerative diseases.

Dr. Li and her team have created several multi-faceted and integrated MS-based platforms that include high resolution *in-situ* peptide mapping, tissue imaging, *in vivo* microdialysis, high sensitivity micro-separation techniques coupled with tandem MS *de novo* sequencing, and new isotopic and isobaric labeling strategies, and improved bioinformatics tools to allow large-scale discovery and functional analysis of novel neuropeptides. More recently, the Li group also employed novel use of ion mobility MS to address several remaining technical challenges associated with peptidomic research. They developed a novel site-specific strategy to rapidly and precisely localize peptide epimers and new strategies to probe peptide sequence scrambling and peptide misidentification, and to improve isobaric tandem mass tag quantitation in QTOF based instrumentation.

Using these integrated platforms and multifaceted approaches, Professor Li and her group discovered more than 300 novel neuropeptides in crustacean model organisms whose genomic sequences are currently unavailable. These findings significantly expanded our knowledge about neuropeptides in these important model organisms and transformed current understanding of neuropeptide family organization and functional consequences of neuropeptide multiplicity.

Dr. Li is Professor of Pharmaceutical Sciences and Chemistry at the University of Wisconsin-Madison.

2014 RESEARCH AWARDS



The Research Awards are fully funded by Thermo Scientific and Waters Corporation in the amount of \$35,000 each. Awards will be presented at the Biemann Medal Award Lecture, 4:45 pm, Tuesday, Exhibit Hall AB, level 1

Sponsored by
THERMO SCIENTIFIC



Kerri A. Pratt
University of Michigan

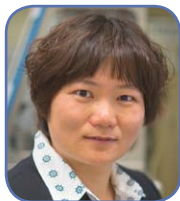
Sponsored by
WATERS CORPORATION



Zhibo Yang
University of Oklahoma

2014 POST-DOCTORAL AWARDS

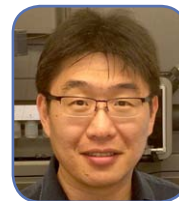
ASMS inaugurates the Post-Doctoral Awards in 2014. Three awards in the amount of \$10,000 each will be awarded annually. The purpose of the award is to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities envisioned for this award include, but are not limited to, conference and workshop attendance, travel to other mass spectrometry laboratories, purchase of books and/or software. The awards are open to ASMS members who are postdoctoral fellows within three years of completing a Ph.D. or equivalent degree. Applicants must be currently appointed as a postdoctoral fellow in North America (e.g., in academia, industry, a government or national laboratory or at a research institute). Details and an application are posted to asms.org.



Huilin Li
University of California, Los Angeles



Boone Prentice
Vanderbilt University



Hao Zhang
Washington University at St Louis

RON A. HITES AWARD FOR OUTSTANDING RESEARCH PUBLICATION IN JASMS



The Ron Hites Award recognizes an outstanding presentation of original research. Selection is based on a paper's innovative aspects, technical quality, likely stimulation of future research, likely impact on future applications, and quality of presentation. The award is named in honor of Professor Ron Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS. The corresponding author receives a cash award of \$2,000 and all authors are acknowledged with certificates of commendation.

The 2014 award recognizes **Evan Williams** and co-authors Harry J. Sterling; Alexander F. Kintzer; Geoffrey K. Feld; Catherine A. Cassou; Bryan A. Krantz; for their paper **Supercharging Protein Complexes from Aqueous Solution Disrupts their Native Conformations**; *JASMS* 2012, vol. 23, pages 191 – 200.

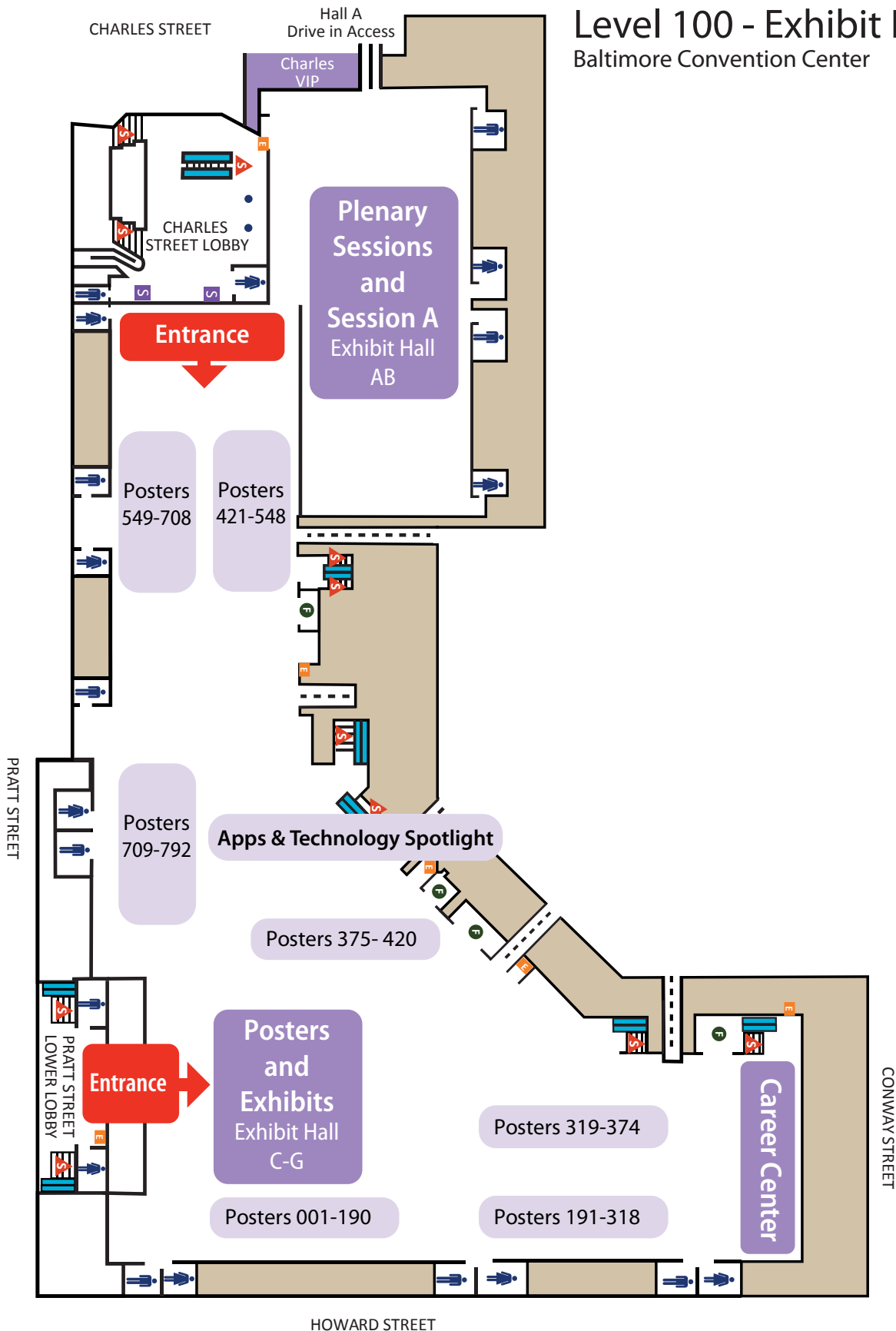


Left to right: Alexander F. Kintzer, Geoffrey K. Feld, Brian A. Krantz, Evan R. Williams, Catherine A. Cassou, and Harry J. Sterling



Level 100 - Exhibit Halls

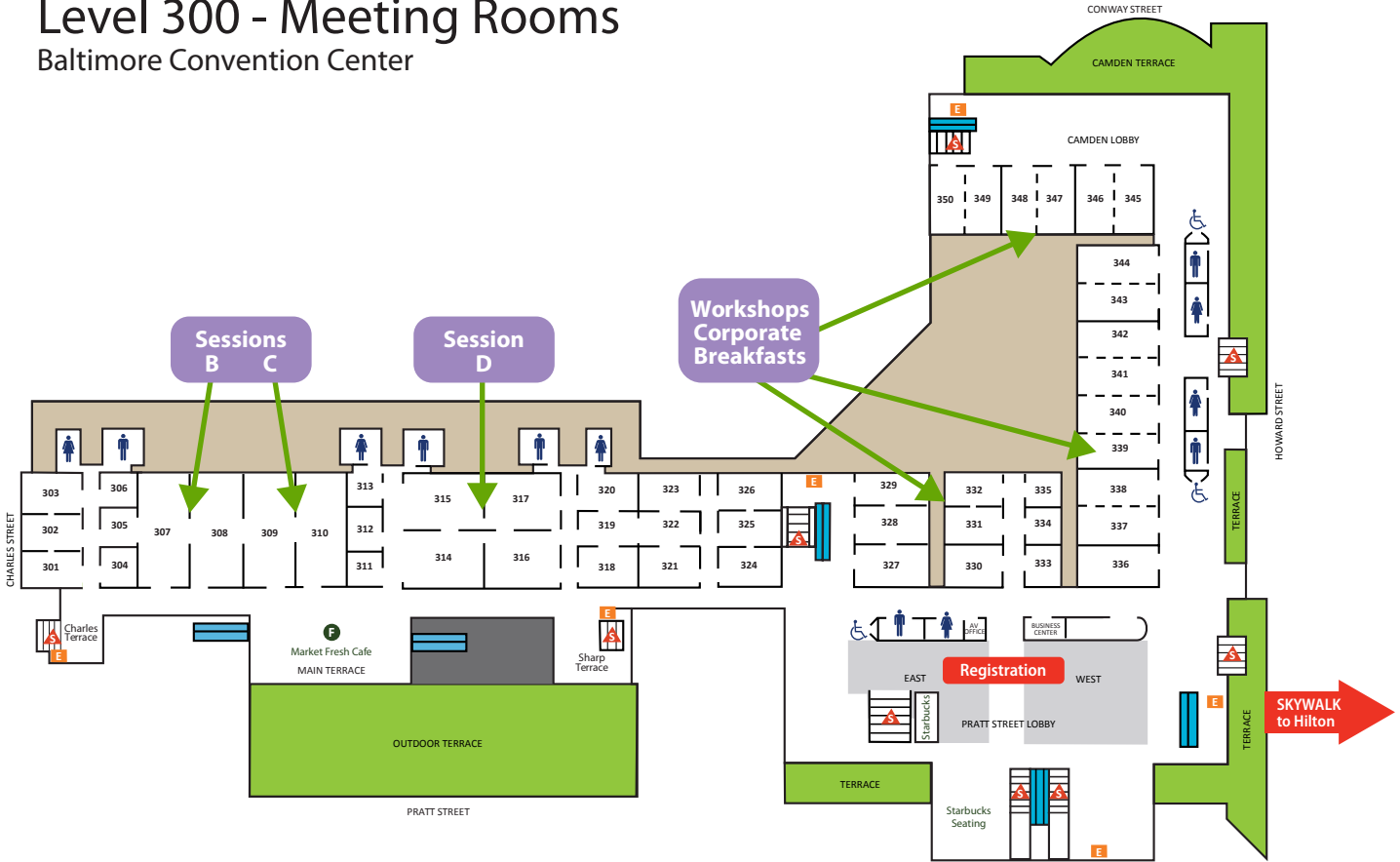
Baltimore Convention Center





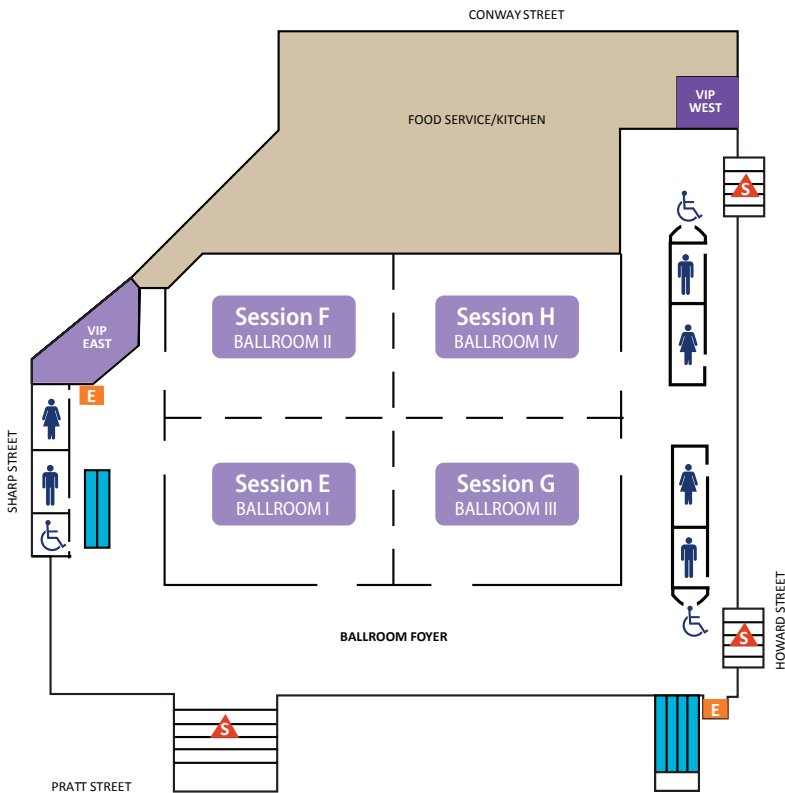
Level 300 - Meeting Rooms

Baltimore Convention Center



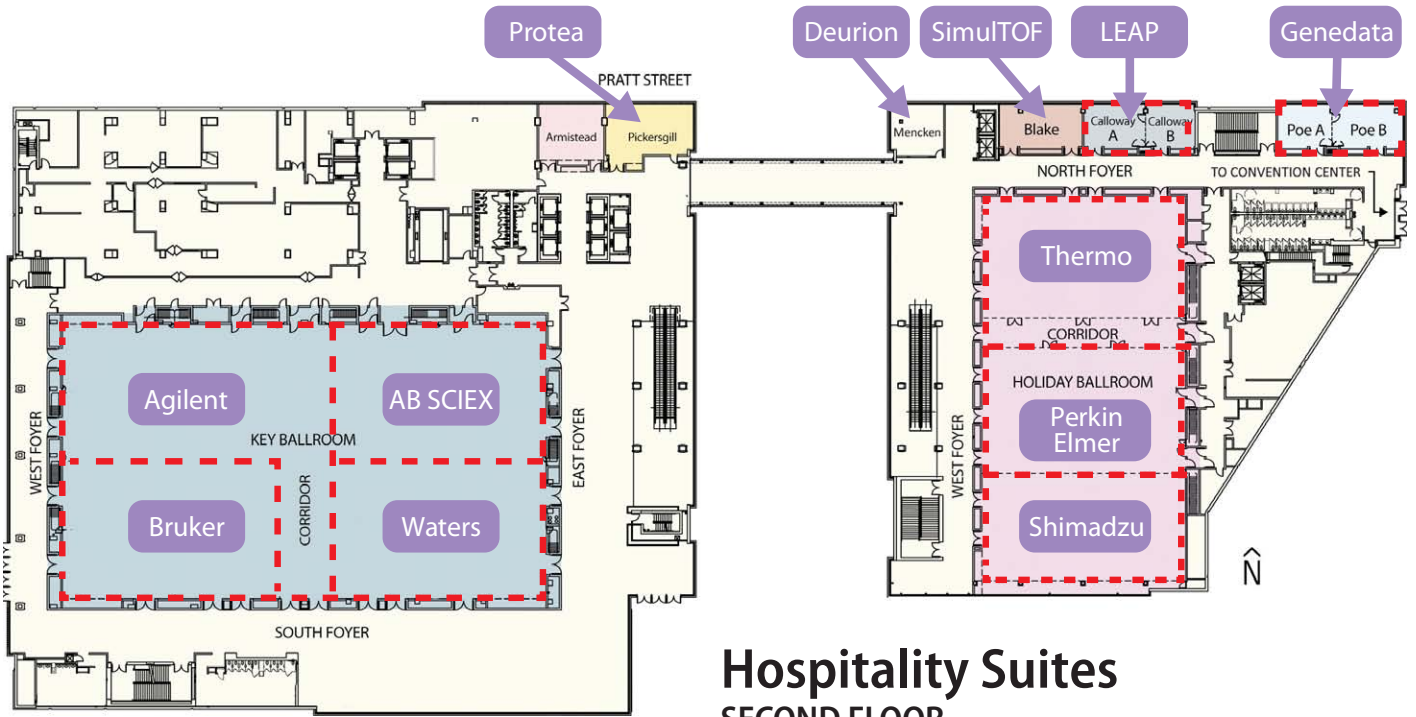
Level 400 - Ballroom

Baltimore Convention Center

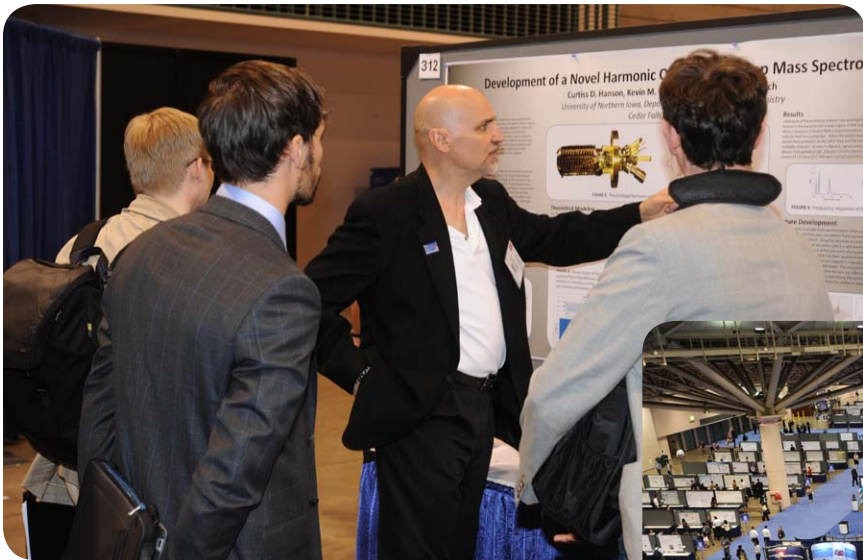




HOSPITALITY SUITES IN HILTON HOTEL



Hospitality Suites SECOND FLOOR Hilton Hotel



ASMS CORPORATE MEMBERS



Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
AB SCIEX	160		Key 7	Rm 343/344, Mon-Wed; Rm 345/346 Mon-Tues; Rm 347/348 Mon
Advanced Chemistry Development (ACD/Labs)	36	Poster		Room 328, Mon
Advion	176			
Agilent Technologies	84	Poster	Key 5	Room 339/340, Mon-Wed
AIM Research Company	2			
Alliance Pharma, Inc.	171			
Analytical Chemistry		Library		
Analytical Sales & Services	87	Poster		
Anasys Instruments	12			
Antec	180	Poster		
Apricot Designs, Inc.	76			
Avanti Polar Lipids, Inc.	174			
Bertin Technologies	17			
BIOCRATES Life Sciences	143			
Bioinformatics Solutions Inc.	42	Poster		
Bioreclamation/VT	77			
Biotage	33			
Biotech Support Group	58			
Bonna-Agela Technologies Ltd.	149			
Bruker Daltonics	49		Key 6	Room 338, Mon-Wed
C&EN	155			
CAMAG Scientific, Inc.	109			
Cambridge Isotope Labs	62			
Canadian Life Science	141	Poster		
Cell Signaling Technology	15			
Cerilliant		Poster		
Cerno Bioscience	63			
Chemyx, Inc.	137			
CovalX	28			
CSS Analytical Co., Inc.	34			
CTC Analytics	93			
Denator AB	20			
Detector Technology, Inc.	72			
Deurion		Poster	Mencken	
Digital Proteomics		Poster		
Drummond Scientific	179			
Edwards	164			
EMCO High Voltage Corporation	133			
EMD Millipore	40	Poster		Room 336, Mon
ES Industries	75	Poster		
ESI Source Solutions		Poster		
ETP Electron Multipliers	124			
Exelis	55	Poster		



ASMS CORPORATE MEMBERS

Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
Extrel CMS	99	Poster		
F.DGSI	102			
FLIR Systems, Inc.	73	Poster		
Fluid Management Systems	165	Poster		
Frontage Laboratories, Inc.	26			
Genedata	57		Poe	
Genetic Engineering & Biotechnology News		Library		
Genovis	126	Poster		
GenTech Scientific Inc.	48			
GERSTEL, Inc.	71	Poster		
GL Sciences	111			
Glygen Corp.	106	Poster		
Golden West Biologicals	154			
Hamamatsu Corporation	39	Poster		
Hamilton Robotics	7			
Harvard Apparatus	122			
HiTek Power	50			
Horizon Technology, Inc.	123			
HTX Technologies, LLC	136	Poster		
Hudson Surface Technology	53	Poster		
iChrom Solutions	103			
IDEX Health & Science	56	Poster		
Imtakt USA	150			
Institute for Systems Biology	5			
INTAVIS, Inc.	91			
Integrated Analysis, Inc.	30	Poster		
Integrated Proteomics Applications	25			
International Equipment Trading Ltd	115			
International Labmate		Library		
ionBench	140			
IONICS Mass Spectrometry	151			
IonSense, Inc.	120	Poster		
IROA Technologies		Poster		
IsoSciences, LLC	145			
JEOL USA, Inc.	107			
JPT Peptide Technologies	97			
LEAP Technologies	14	Poster	Calloway	
LECO Corporation	92	Poster		Room 327, Mon-Wed
LNI Schmidlin	105			
M&M Mass Spec Consulting	128			
Mac-Mod Analytical	96			
MassTech, Inc.	29			
Matrix Science	22			
McKinley Scientific	89			
MestreLab Research	132			

ASMS CORPORATE MEMBERS



Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
Metabolon, Inc.	156	Poster		
Microliter Analytical Supplies	16			
Microsaic Systems PLC.....	74	Poster		
Moeller Medical GmbH.....	59			
Molecular & Cellular Proteomics		Library		
Morpho Detection Inc.	44	Poster		
MS Bioworks.....	79			
MS Noise.....	35			
MS Vision	138			
MSParts Inc.....	90			
mSPEC Group.....	95			
nanoLiter, LLC	135	Poster		
Nest Group, The		Poster		
New England Peptide.....	82			
New Objective, Inc.....	88	Poster		Room 328, Tues
NIST	125			
Norgren, Inc.....	130	Poster		
Oerlikon Leybold Vacuum.....	104			
OI Analytical.....	166			
Omni Enclosures	38			
Omni International	8	Poster		
Optimize Technologies	54	Poster		
Owlstone, Inc.....	117			
Parker Hannifin.....	70	Poster		
PEAK Scientific.....	119	Poster		
Perfinity Biosciences, Inc.....	159	Poster		
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ASMS CORPORATE MEMBERS

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PROGRAM ACKNOWLEDGEMENTS



Jenny Brodbelt
University of Texas, Austin
Vice President for Programs

STUDENT ASSISTANTS

Graduate students assist with many aspects of the conference, including registration, oral and poster sessions, and the Career Center. The students each receive a stipend to help with their conference travel expenses.

PROGRAM COMMITTEE

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Victoria Cotham		Junmei Zhang

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Matt Crowe	Chris Gill	Richard Perry	Renato Zenobi

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Olga Friese	Liam McDonnell	Don Smith	Ralf Zimmerman






PROGRAM OVERVIEW

SATURDAY

9:00 AM - 4:30 PM	SHORT COURSES
2:00 - 5:00 PM	REGISTRATION

SUNDAY

9:00 AM - 4:30 PM	SHORT COURSES
10:00 AM - 8:00 PM	REGISTRATION
5:00 - 6:30 PM	<p>TUTORIAL LECTURES, Exhibit Hall AB, level 1</p> <div style="display: flex; flex-direction: column; gap: 10px;"> <div style="display: flex; align-items: center;">  <div style="margin-left: 10px;"> <p>5:00 - 5:45 pm Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know But Were Afraid to Ask</p> <p>Lucinda Cohen Merck Research Laboratories</p> </div> </div> <div style="display: flex; align-items: center;">  <div style="margin-left: 10px;"> <p>5:45 - 6:30 pm Imaging Mass Spectrometry</p> <p>Ron M.A. Heeren FOM-AMOLF</p> </div> </div> </div>
6:45 - 7:45 PM	<p>CONFERENCE OPENING, Exhibit Hall AB, level 1 Jenny Brodbelt, ASMS Vice President for Programs</p> <div style="display: flex; align-items: center; margin-top: 10px;">  <div style="margin-left: 10px;"> <p>7:00 - 7:45 pm</p> <p>The James Webb Space Telescope: From First Light to the Search for Earth 2.0</p> <p>Jason Kalirai Telescope Science Institute</p> </div> </div>
7:45 - 9:00 PM	RECEPTION IN THE POSTER-EXHIBIT HALL

SPACEFLIGHT MASS SPECTROMETRY 1963 – 2018

A small exhibit featuring models of spaceflight mass spectrometers employed in the exploration of the Solar System over the past several decades is displayed in the Pratt Lobby. Mass spectrometers have contributed substantially to our understanding of planetary science and astrobiology, and their continued use has a bright future with new technologies under development. Displayed models



include engineering units, flight spares, and demonstration reproductions from robotic planetary missions to Venus, Jupiter, Saturn, Titan, and Mars. Experts will be on hand to answer questions about instrument design, mission science achievements, and future direction associated with these one-of-a-kind instruments.

The display has been coordinated by William B. Brinckerhoff, NASA GSFC, Greenbelt MD.



PROGRAM OVERVIEW



MONDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • MOA am: Emerging Environmental Contaminants, Exhibit Hall AB, level 1 • MOB am: Instrumentation: New Developments in High Resolution and Mass Accuracy to Celebrate Alan Marshall's 70th Birthday, Room 307-308, level 3 • MOC am: Nucleic Acids, Room 309-310, level 3 • MOD am: Fundamentals: Reactions, Dynamics and Theory of Gas Phase Ions, Room 314-317, level 3 • MOE am: Antibodies and Antibody-Drug Conjugates, Ballroom I, level 4 • MOF am: H/D Exchange: New Developments in Technology, Ballroom II, level 4 • MOG am: Informatics: Protein Identification, Ballroom III, level 4 • MOH am: PTMs: Advances in Isolation, Enrichment, Derivatization and Separation, Ballroom IV, level 4
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Poster/Exhibit Hall, level 1</p> <p>Monday posters</p> <p>12:00 – 1:00 pm: Undergraduate students – look for reserved tables to <i>Meet the Experts</i></p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • MOA pm: Polymer- and Packaging-Related Contaminants and Degradants in Consumer Products, Exhibit Hall AB, level 1 • MOB pm: Instrumentation: Mini/Portable/Fieldable Mass Spectrometry, Room 307-308, level 3 • MOC pm: Ion Mobility: Structures to Celebrate Mike Bowers' 75th Birthday, Room 309-310, level 3 • MOD pm: Photoionization, Room 314-317, level 3 • MOE pm: Characterization of Biologics and Biosimilars, Ballroom I, level 4 • MOF pm: Quantitative Analysis in Drug Discovery and Development, Ballroom II, level 4 • MOG pm: Informatics: Protein Quantification, Ballroom III, level 4 • MOH pm: Imaging: Biomedical Applications, Ballroom IV, level 4
4:45 - 5:30 PM	<p>AWARD LECTURE, Exhibit Hall AB, level 1</p> <div style="display: flex; align-items: center;">  <div> <p>Award for a Distinguished Contribution in Mass Spectrometry</p> <p>Richard M. Caprioli Vanderbilt University</p> </div> </div>
5:45 - 7:00 PM	<p>WORKSHOPS All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> 1. Real World Applications of Photoionization; Room 307-308 2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group); Room 309-310 3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Room 314-317 4. How to Succeed in Pharma without Really Trying; Room 327 5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group); Room 336 6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum & Biofuels Interest Group); Room 337 7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); Room 338 8. ProteomicsDB; Room 339-340 9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Room 341-342 10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry (organized by Lipids and Lipidomics Interest Group); Room 343-344 11. A State of the Union for Biomarker Translation (organized by Clinical Chemistry Interest Group); Room 345-346 12. Antibody Drug Conjugates as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Room 347-348 13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security (organized by Forensics and Homeland Security Interest Group); Room 349-350
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Hilton Hotel

PROGRAM OVERVIEW

TUESDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • TOA am: Integrated Qualitative and Quantitative LC-MS for Small Molecule Analysis, Exhibit Hall AB, level 1 • TOB am: Instrumentation and Methods: FT, Ion Traps and Hybrid Instruments, Room 307-308, level 3 • TOC am: Ion Mobility: Separations, Room 309-310, level 3 • TOD am: Macromolecular Complexes: Activation and Dissociation, Room 314-317, level 3 • TOE am: PK/PD Analysis of Biologics, Ballroom I, level 4 • TOF am: H/D Exchange: Biological Applications, Ballroom II, level 4 • TOG am: Phosphoproteomics in Disease, Ballroom III, level 4 • TOH am: Imaging: Pharmaceuticals and Metabolomics, Ballroom IV, level 4
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Poster/Exhibit Hall Tuesday posters
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • TOA pm: Space Science, Astrobiology, and Atmospheric Chemistry, Exhibit Hall AB, level 1 • TOB pm: Nano-Scale and Microfluidic Separations and Mass Spectrometry, Room 307-308, level 3 • TOC pm: Protein-Protein and Protein-Ligand Interactions, Room 309-310, level 3 • TOD pm: Fundamentals of Peptide Fragmentation, Room 314-317, level 3 • TOE pm: Top-Down Protein Analysis, Ballroom I, level 4 • TOF pm: Drug Target Discovery and Validation, Ballroom II, level 4 • TOG pm: Clinical Diagnostics, Ballroom III, level 4 • TOH pm: Imaging: Fundamentals, Instrumentation, and Method Development, Ballroom IV, level 4
4:45 - 5:30 PM	<p>AWARD LECTURE, Exhibit Hall A/B (lower level)</p>  <p>Biemann Medal</p> <p>Lingjun Li University of Wisconsin-Madison</p>
5:45 - 7:00 PM	<p>WORKSHOPS All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> 1. H/D Exchange, Covalent Labeling and Crosslinking (organized by H/D Exchange, Covalent Labeling & Cross Linking Interest Group); Room 307-308 2. LC-MS System Performance Tracking in LC-MS Tracking in LC-MS (organized by LC/MS & Related Topics Interest Group); Room 309-310 3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis (organized by Regulated Bioanalysis Interest Group); Room 314-317 4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment (organized by Analytical Lab Managers Interest Group); Room 336 5. FTMS: ICR and Orbitrap (organized by FTMS Interest Group); Room 337 6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry (organized by Environmental Applications Interest Group); Room 338 7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess (organized by Fundamentals Interest Group); Room 339-340 8. The NIH Review Process and Mock NIH Study Section; Room 341-342 9. Imaging Mass Spectrometry vs. Histology (organized by Imaging MS Interest Group); Room 343-344 10. Metabolomics: Emerging Technologies for Continued Innovation (organized by Metabolomics Interest Group); Room 345-346 11. 50 Years of the British Mass Spectrometry Society: Past, Present & Future; Room 347-348 12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud; Room 349-350
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Hilton Hotel

PROGRAM OVERVIEW



WEDNESDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • WOA am: Energy, Petroleum, and Biofuels: Advances in Sample Preparation and MS Interface Design, Exhibit Hall AB, level 1 • WOB am: Ambient and Atmospheric Pressure Ionization: Fundamentals, Room 307-308, level 3 • WOC am: The Triple Quadrupole: 35 Years of Evolution and Application to Celebrate Chris Enke's 80th Birthday, Room 309-310, level 3 • WOD am: Quantitative Proteomics in Systems Biology/Cellular Pathway Analysis, Room 314-317, level 3 • WOE am: Peptidomics, Ballroom I, level 4 • WOF am: Pharmacoproteomics and Toxicoproteomics for Drug Development, Ballroom II, level 4 • WOG am: PTMs: Comprehensive Analysis, Ballroom III, level 4 • WOH am: Lipids and Profiling, Ballroom IV, level 4
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Poster/Exhibit Hall Wednesday posters</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <ul style="list-style-type: none"> • WOA pm: Energy, Petroleum, and Biofuels: Advances in MS Design and Informatics, Exhibit Hall AB, level 1 • WOB pm: Ambient Ionization: Instrumentation and Applications, Room 307-308, level 3 • WOC pm: Ecological and Human Health Environmental Chemistry and Toxicology, Room 309-310, level 3 • WOD pm: Fundamentals: New Ion Activation Methods, Room 314-317, level 3 • WOE pm: Plant "omics", Ballroom I, level 4 • WOF pm: Proteomics: Infectious Diseases, Ballroom II, level 4 • WOG pm: Targeted Quantification of Proteins and Post-translational Modifications, Ballroom III, level 4 • WOH pm: Membrane Proteins, Ballroom IV, level 4
4:45 - 5:30 PM	ASMS MEETING , Ballroom I, level 4 Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	<p>WORKSHOPS All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> 1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Room 307-308 2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Room 309-310 3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Room 314-317 4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Room 336 5. Have Quadrupole Ion Traps Passed their Prime Time? (organized by Ion Trap Interest Group); Room 337 6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Room 338 7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Room 339-340 8. Using Mass Spectrometry to Characterize the Exposome and Its Impact on Human Health; Room 341-342 9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message; Room 343-344 10. Quantitative Glycomics; Room 345-346 11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS; Nalini Sadagopan, Room 347-348 12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS (organized by Flavor Fragrance and Foodstuff Interest Group); Room 349-350 13. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 327
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Hilton Hotel

PROGRAM OVERVIEW

THURSDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS <ul style="list-style-type: none"> • ThOA am: Forensic Applications, Exhibit Hall AB, level 1 • ThOB am: Instrumentation: New Developments in Ionization and Sampling, Room 307-308, level 3 • ThOC am: FAIMS and DMS: New Developments and Applications, Room 309-310, level 3 • ThOD am: Radical Ion Chemistry, Room 314-317, level 3 • ThOE am: Biomarkers in Drug Discovery, Development and Diagnosis, Ballroom I, level 4 • ThOF am: Covalent Labeling, Chemical Probes, and Crosslinking for Biomolecule Structural Characterization, Ballroom II, level 4 • ThOG am: Informatics: Metabolomics, Ballroom III, level 4 • ThOH am: Glycoproteins and Glycans: New MS Approaches, Ballroom IV, level 4
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Poster/Exhibit Hall Thursday posters
2:30 - 4:30 PM	ORAL SESSIONS <ul style="list-style-type: none"> • ThOA pm: Food Chemistry and Safety, Exhibit Hall AB, level 1 • ThOB pm: Instrumentation: Time-of-Flight Mass Spectrometry, Room 307-308, level 3 • ThOC pm: Mass Spectrometry in Structural Biology, Room 309-310, level 3 • ThOD pm: Fundamentals: Ion Spectroscopy, Room 314-317, level 3 • ThOE pm: Data Independent Acquisition, Ballroom I, level 4 • ThOF pm: Epigenetic Modifications and Mechanisms, Ballroom II, level 4 • ThOG pm: Metabolomics/Lipidomics: New MS Technologies and Applications, Ballroom III, level 4 • ThOH pm: Carbohydrates: New MS Approaches, Ballroom IV, level 4
4:45 - 5:30 PM	PLENARY LECTURE , Exhibit Hall AB, level 1  <div style="clear: both;"></div> <p style="margin-left: 20px;">How the Genome Folds</p> <p style="margin-left: 20px;">Erez Lieberman Aiden Baylor College of Medicine and Rice University</p>
6:30 - 9:00 PM	CLOSING EVENT, National Aquarium. Ticket required

All workshops are located on level 3. There are light refreshments on level 3.

MONDAY WORKSHOPS, 5:45 - 7:00 PM

1. Real World Applications of Photoionization;

Ralf Zimmerman and Jack Syage presiding
Room 307-308

The workshop on Photoionization last year was a success with a standing room only crowd to the end. That workshop brought the mechanism of atmospheric pressure photoionization and vacuum photoionization up to date and stimulated significant discussion. This year we would like to focus more on applications as PI is expanding in its uses ranging from APPI in LC/MS in petroleums, food safety, and environmental monitoring to ambient analysis (DAPPI, DART/APPI, etc.) to its now becoming the preferred ionization source for explosives detection airport security detection systems (MS and IMS) potentially expanding the user base by yet another few thousand. This would be a great opportunity to get discussion and feedback on these new developments from the MS community and perhaps set the stage for a PI oral session in 2015 as these new developments mature.

2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group);

Karl Clauser, Karl Mechtler, Lukas Käll, David Tabb presiding
Room 309-310

The use of database search engines for identification of posttranslational modifications (PTMs) is common practice in most proteomics labs, but these identifications have been plagued by errors from two key sources. Karl Clauser will highlight the elevation of false discovery rates that results from allowing more degrees of freedom in identification, such as allowing for "blind PTM" searches or permitting too many modifiable sites in some peptides. Karl Mechtler will emphasize localization, the challenge of associating PTMs with the appropriate residue when multiple modifiable sites may be found in a peptide. Which PTM challenge merits more attention from the bioinformatics research community?

3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Matthew Bush and Erin Baker presiding

Room 314-317

Results from ion mobility mass spectrometry studies are increasingly used to answer questions in biology, including applications to metabolomics, proteomics, targeted interactions, and large molecules. This is in part attributed to the increasing performance and selection of commercial ion mobility mass spectrometry instrumentation, which has made it easier to integrate ion mobility technologies into mass spectrometry workflows. In this workshop, we will showcase research that demonstrates the advantages of ion mobility for biological applications. There will also be opportunities to discuss the challenges that arise in different types of ion mobility studies, what is possible today, and opportunities for the future.

4. How to Succeed in Pharma without Really Trying;

Lucinda Cohen presiding
Room 327

This workshop will focus on advice to young scientists considering career choices after graduation. An expert panel consisting of current and former pharmaceutical scientists will engage in dialogue with the audience around their experiences job-hunting, changing positions, networking inside and outside the company, and thriving in today's ever-changing environment. Audience participation will be an essential driver for the workshop, with shared participant experiences being welcome. This workshop will continue the theme of the Sunday Tutorial Lecture by Lucinda Cohen, "Everything You Ever Wanted to Know about Mass Spectrometry in the Pharmaceutical Industry but Were Afraid to Ask." However, the focus will be pragmatic and offer insider perspectives on life in an industrial laboratory environment. Ultimately the intent is to help young mass spectrometrists connect with pharmaceutical industry veterans.

5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group);

Norman Chiu and Michael McGinley presiding
Room 336

The workshop will cover recent advances in MS characterization of oligonucleotides with an emphasis on recent development in sample preparation as well as MS data processing. While MS instrument development will likely be covered in other sessions, there have been several developments both in sample preparation of oligonucleotides as well as data analysis of collected data. The proposed workshop will have 4 short topic "primers" from thought leaders starting discussions; two about sample processing leading to oligonucleotide analysis using MS/MS as well as two discussing data interpretation of MS/MS data for oligonucleotides. Discussion should lead to some view of the current trends in analysis of oligonucleotides by MS.

6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum & Biofuels Interest Group); Patrick Hatcher and Lateefah Stanford presiding

Room 337

The molecular complexity of biofuels and petroleum has offered an analytical challenge for those interested in assessing their composition. Advances in 2 dimensional GC x GC-MS, Fourier transform MS and Ion mobility MS are allowing for an exhaustive molecular characterization of these materials, to the point that a comprehensive molecular-level characterization of these mixtures is within reach. New developments in MS instrumentation and approaches are paving the way for advanced characterization of complex mixtures like petroleum and biofuels. The workshop will invite discussion leaders at the forefront of applications of these advanced MS approaches in the energy field to enlighten interested groups to venture into the arena.

7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); JC Poutsma and Elaine Marzluff presiding

Room 338

Panel discussion with current undergrads, recent graduates, and faculty members at PUI institutions. This workshop is designed for undergraduates who are attending the ASMS meeting and will focus on how best to leverage their undergraduate research into success in graduate school and industry.

8. ProteomicsDB; Bernhard Kuster and Mathias Wilhelm presiding

Room 339-340

There is a growing landscape of various databases and repositories for MS and proteomics. In this workshop, we would like to present ProteomicsDB, a free, professionally developed solution to store and analyze mass spectrometry-based proteomics data. ProteomicsDB has a strong focus on functionality and secondary use of proteomics and mass spectrometry data. We would like to discuss our motivations for initiating this effort, demonstrate typical use-cases for web interface and API, describe our short and long-term plans and generally encourage the involvement from the ASMS community.

9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Douglas Sheeley, Charles Edmonds,

and Salvatore Sechi presiding
Room 341-342

A major source of financial support for US research is the federal government. Unfortunately, researchers are sometimes not aware of the resources available to them. This two session workshop, to be held on consecutive evenings at the ASMS conference, will discuss the identification of appropriate agencies and programs, writing an effective application, responding to the criticisms of reviewers, and taking full

MONDAY WORKSHOPS, 5:45 - 7:00 PM continued

advantage of guidance from program administrators. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on the new investigator. References to additional resources will be provided. A "mock" NIH study section presentation will provide additional insight into the review process at that agency, and an opportunity for discussion with NIH staff. Each session will allow substantial time for questions and staff will be available for one-on-one conversations afterward on both evenings.

10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry (organized by Lipids and Lipidomics Interest Group); Stephen Blanksby and Christer Ejsing presiding
Room 343-344

The 61st ASMS conference in Minneapolis played host to the first workshop on "Lipid Mass Spectrometry and Lipidomics". This workshop was attended by ~190 participants and resulted in vibrant discussion. A recurring theme was the importance of developing guidelines for the uniform reporting of mass spectrometry-based lipid and lipidome data, particularly in terms of an abbreviation code that encapsulates the exact level to which lipids can be structurally defined and/or quantified when using a particular MS or MS/MS approach. This workshop will invite opinion on systems of annotation and reporting requirements from leaders in the field that will then be opened for discussion and input from all workshop participants. An expected outcome of this workshop will be the formation of a working group to collate and consider the ideas presented and to refine this into a series of recommendations for lipid mass spectrometrists.

11. A State of the Union for Biomarker Translation (organized by Clinical Chemistry Interest Group); Brian Rappold and Cory Bystrom presiding
Room 345-346

With recent announcements from CPTAC and commercial companies that are offering novel diagnostics derived from proteomics research this presents an opportunity to review the problems that have been solved and the challenges that lie ahead. In this workshop, we will invite several guest speakers to give a brief assessment of the landscape from discovery to clinical utilization/commercialization which

will be followed by a moderated discussion. The co-chairs will also be soliciting ideas for future workshop topics so bring your ideas.

12. Antibody Drug Conjugates as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Brian Furmanski and Shawna Hengel presiding
Room 347-348

Due to the success of the 2013 pharmaceutical interest group workshop we will continue with a similar format being; the overview of the topic of antibody drug conjugates as pharmaceutical agents with a short informal presentation (10 min) by an academic/industrial leader. Following the presentation the panelists will be introduced along with three key questions to start of the discussion with the general audience. The short presentation is meant to capture the field in its current state, in addition give specific examples of challenging issues in the industry for the discovery and development of antibody drug conjugates. Potential areas of discussion may include characteristics of antibodies, drug antibody ratio (DAR) in vivo/ex vivo, strategies for sample prep/isolation, choice of mass analyzers and a comparison of complimentary tools to mass spectrometry including: ELISA, Luminex, page electrophoresis, Edman sequencing and surface plasmon resonance. To identify panelists, gauge the level of interest of the ASMS community and to tailor the discussion we will send out a survey of open ended questions in April.

13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security (organized by Forensics and Homeland Security Interest Group); Guido Verbeck and Glen Jackson presiding
Room 349-350

Forensic-related applications of mass spectrometry has some unique challenges for researchers wishing to pursue a career in this field. We plan to stimulate an informative discussion between roundtable participants and audience members around the following topics: Funding; publishing; collaborating; job hunting; academic challenges. Roundtable participants will include knowledgeable and experienced members of the forensic and homeland security community, including representatives of funding agencies, crime labs, academia and publishers.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM

All workshops are located on level 3. There are light refreshments on level 3.

1. H/D Exchange, Covalent Labeling and Crosslinking (organized by H/D Exchange, Covalent Labeling & Cross Linking Interest Group); Joshua Sharp and David Schriemer presiding
Room 307-308

The workshop will provide a forum for discussing the latest HDX, covalent labeling and crosslinking methods for protein analysis. Presentations will provide an opportunity to discuss MS-based methods, data analysis routines and applications with the attendees. The goal of these presentations will be to stimulate discussion and convey useful experimental detail you can take back to your lab.

2. LC-MS System Performance Tracking in LC-MS (organized by LC/MS & Related Topics Interest Group); Helene Cardasis presiding
Room 309-310

While this group has previously hosted an annual workshop on LC-MS troubleshooting, this year we will take a more preventative approach. The workshop this year will focus on important aspects of whole-platform performance tracking with respect to defining data quality, understanding performance drift, and facilitating/ expediting troubleshooting when issues do arise. Discussion will touch on choice of QC sample, instrument method, frequency of measurement, key metrics and their interpretation, and QC data processing. We will also review and demo some of the freeware available for this purpose. As always, audience participation in the form of both questions and heated debate are encouraged!

3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis (organized by Regulated Bioanalysis Interest Group); Fabio Garofolo and Keyang Xu presiding
Room 314-317

The purpose of this workshop is to provide an informal venue for the discussion of ADCs from a Regulated Bioanalytical point of view based on recent industry consensus. Dr. Keyang Xu (Genentech) will lead the discussion together with a recognized panel of bioanalytical experts in the field. As per the ASMS workshop format there will not be formal presentations but the participants will introduce the discussion topics for maximum of 10 minutes to engage the audience and encourage all to participate in a dynamic and productive discussion.

ADCs are generally complex heterogeneous mixtures of multiple species, these novel therapeutic products present unique challenges in Regulated Bioanalysis: Heterogeneity of the reference material (e.g.: lysine side chain-based conjugation; hydrazine-based); Heterogeneity impact on assay accuracy; In-vivo dynamicity and deconjugation (mixture of DAR); LC-MS high sensitivity for unconjugated drug detection. Multiple validated methods are need for well characterizing ADCs quantitation: Total antibody; Conjugated antibody; Antibody-conjugated drug; unconjugated/deconjugated drug. Interpretation of the bioanalytical data from these multiple assays can be complex. Discussion will also focus on regulatory expectations surrounding comparability studies for ADC.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment (organized by Analytical Lab Managers Interest Group); Brett S. Phinney and Chris Colangelo presiding

Room 336

Along with a panel of invited laboratory managers, we propose to discuss several topics related to controlling and measuring variation in sample preparation and Data analysis. These topics may include

- 1) How do you control variation in sample preparation
- 2) How do you measure variation in sample preparation
- 3) How to choose an appropriate QC standard, where to buy it or make it if necessary.
- 4) How to determine the appropriate number of replicates you need?
- 5) How to determine what amount of variation is due to sample preparation or biology
- 6) How do you control for variation in data analysis.
- 7) How to document variation and present it to core clientele

The session will discuss practical real world examples and implementations to measure and control for variation in core facilities. Audience members are encouraged to share their struggles and approaches for used in their own laboratories.

5. FTMS: ICR and Orbitrap (organized by FTMS Interest Group); Nathan Kaiser and Don Smith presiding

Room 337

Recent advances in high resolution FTMS have focused on electric field control (e.g. high field Orbitrap and compensated/harmonized ICR cells) and new implementations of advanced data processing (e.g. absorption mode and eFT). These, as well as other new developments in FTMS instrumentation and fundamentals will be discussed. Fundamental and practical topics, as well as current instrument limitations will be open for interactive discussion.

6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry

(organized by Environmental Applications Interest Group); Kerry Peru and Chris Gill presiding

Room 338

Rapid expansion of hydrocarbon extraction, production and processing from nonconventional sources such as shale gas and oil sands has led to the need of determining the industry's impact on the environment by characterizing and monitoring associated contaminants. This year's Workshop is a continuation of last year's topic which drew considerable interest. Updates on analytical methodologies used for monitoring, identification and characterization of contaminants will be discussed along with an update of the state of the industry from an environmental perspective.

7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess (organized by Fundamentals Interest Group);

George Khairallah and Jos Oomens presiding
Room 339-340

This year marks a milestone for several researchers in the fundamentals field including Professor John Bartmess. We plan to honor this special occasion by providing a series of invited short presentations and discussions mainly in the research areas in which John was very active. In the yearly tradition of the fundamentals group, senior graduate students and postdoctoral scholars in research groups will give the presentations.

8. The NIH Review Process and Mock NIH Study Section; Douglas Sheeley, Charles Edmonds, and Salvatore Sechi presiding

Room 341-342

A major source of financial support for US research is the federal government. Unfortunately, researchers are sometimes not aware of the resources available to them. This two session workshop, to be held on consecutive evenings at the ASMS conference, will discuss the

identification of appropriate agencies and programs, writing an effective application, responding to the criticisms of reviewers, and taking full advantage of guidance from program administrators. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on the new investigator. References to additional resources will be provided. A "mock" NIH study section presentation will provide additional insight into the review process at that agency, and an opportunity for discussion with NIH staff. Each session will allow substantial time for questions and staff will be available for one-on-one conversations afterward on both evenings.

9. Imaging Mass Spectrometry vs. Histology (organized by Imaging MS Interest Group); Liam McDonnell and Zoltan Takats presiding

Room 343-344

The topic for discussion will concern the question of where imaging MS can have an impact in diagnostic and prognostic pathology, and what must be done for it to become a recognized clinical method. In order to encourage open discussion we will include a series of deliberately provocative 5-minute presentations.

- i) Imaging MS can replace histology.
- ii) Histology & diagnostics – mass spectrometrists underestimate its importance.
- iii) What is the added benefit of imaging MS in diagnostics?
- iv) In-surgery, *in-situ* analysis
- v) Open discussion – where can imaging MS make a difference?
- vi) What needs to be done for imaging MS to become a recognized clinical tool?

10. Metabolomics: Emerging Technologies for Continued Innovation (organized by Metabolomics Interest Group);

Sunia Trauger and Gary Patti, presiding
Room 345-346

This workshop will begin with a brief discussion of the most exciting technological advances in the field of metabolomics over the past year. The moderators will highlight 2-3 noteworthy metabolomic publications that they feel are particularly impressive achievements and survey the audience for their opinions. Three-four invited scientists with expertise in the technologies highlighted will serve as panelists and answer questions posed by the moderators and attendees. The workshop will close with a discussion among the panelists on their perspectives of emerging trends and the role that these technologies are playing in future development. Advances intended to be highlighted are: (i) software for post-processing of untargeted metabolomic data, (ii) innovative experimental designs using stable isotopes, (iii) shotgun approaches with ion mobility, and (iv) metabolite identification by *in silico* fragmentation.

11. 50 Years of the British Mass Spectrometry Society: Past, Present & Future; Helen Cooper, Sarah Hart,

and Jackie Moseley presiding
Room 347-348

- Presentation by BMSS President Professor John Monaghan on the history of BMSS.
- Three short talks on breaking developments in MS research from the UK
- BMSS travel grants for members to attend ASMS and plan was to select these talks from the recipients of that funding once allocated.
- Panel Q&A session to discuss future direction of BMSS

12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud; Andrey Bondarenko, Michael MacCoss, Christine Wu, and Nathan Yates presiding

Room 349-350

The sharing, public dissemination, and analysis of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a free, professionally developed solution

TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

to the mass spectrometry field's needs. The application provides a "Google Docs" type interface optimized for mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. Over the last year CHORUS has gained almost 400 users and these users have placed >9,000 mass spectrometry data files into the service. We have learned a lot

from user feedback. We would like to discuss improvements made to CHORUS over the last year and what new analysis capabilities have and are being added. We want to discuss our goals and get feedback from the community on our current and long-term priorities.

WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM

All workshops are located on level 3. There are light refreshments on level 3.

1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Yishai Levin and Will Thompson presiding Room 307

The heated debate over data-dependent (DDA) versus data-independent (DIA) acquisition strategies shows no signs of abating. This workshop will focus on defining the experimental characteristics, specifically related to data acquisition, which would make up the "perfect" strategy for 'omic analyses. Facilitators will prime the discussion with some simple use-cases for 'omics analysis, then experts and novices alike will gather to share views on the most important attributes of data acquisition in this space. The goal of the discussion will then be a critical evaluation of current approaches against that "perfect" strategy, with an eye towards features that should exist in the next generation of tools.

2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Don McKenzie and Mustafa Varoglu presiding Room 309-310

One of the challenges faced by mass spectrometrists is the ability to efficiently gather and process data across multiple software platforms. Many scientists consider the advantages of having multiple types of mass spectrometers to leverage the benefits that each platform provides in data collection. Considerations like ion source diversity, trap vs. ToF vs. triple technology, degree and specificity of product ion formation etc. play into the strategy of building a high quality laboratory. With this in mind, it is common to equip laboratories with instrumentation from various vendors. However, many times a preferred procedure for data collection and/or processing can be limited or unavailable depending upon which vendor based set of hardware is employed. Reasons for this disparity can range from differences in vendor specific software capabilities to data collection and/or processing limitations incurred via patent restrictions. Further, having to train staff in the utilization of the various platforms can be time consuming and tie up limited resources. This workshop will focus on the various mechanisms used across labs to overcome software limitations as well as explore the idea of open source coding for DMPK mass spectrometry data analysis.

3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Li Tao and Arindam Roy presiding Room 314-317

This would be a forum to discuss current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Development of new methodologies to improve efficiency and robustness of mass spectrometric analysis will be discussed in this forum. Background information on several topics will be provided to initiate the discussion. Example of some topics for discussion would be

- (1) Molecular variants analysis
- (2) Degradation pathway identification
- (3) Quantitative analysis of glycosylation
- (4) Improving the speed of LC/MS analysis

4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Olga Friese and Dian Su presiding Room 336

The workshop features a panel discussion on professional development. Topics will be focused on career planning and management, fundamental training, industrial internship, job search tools and interview strategies. The panel, consisting of representatives from government, industrial and academic organizations, will share their knowledge and practices on career prospects.

5. Have Quadrupole Ion Traps Passed their Prime Time? (organized by Ion Trap Interest Group); Yu Xia presiding Room 337

In this workshop we will discuss the current status and possible future advancement of quadrupole ion traps, with relevance to the development of various types of mass analyzers. The following questions will be asked: 1. As a mass analyzer, how will ion traps compete with others and what are the critical technical advancements? 2. Structural confirmation by MS/MS vs. high resolution MS, any chance at all? 3. Ion trap as a reaction/storage vessel – what new capabilities are coming out of in research and what should be transferred to commercial instrument?

6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Gyorgy Vas and William Erb presiding Room 338

This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, products, etc.

7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Tim Griffin presiding Room 339-340

The open source Galaxy software framework is gaining momentum as a tool to solve biological MS informatics problems. It offers unique features such as flexibility to integrate disparate software programs into effective workflows, and the ability to share complete workflows with other researchers. In this workshop, expert developers and users of Galaxy for biological MS data analysis will present practical tutorials. Presentations will be aimed at informing both software developers and biologists/analytical chemists on how they can make effective use of the Galaxy framework in their research.

WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM continued

8. Using Mass Spectrometry to Characterize the Exposome and Its Impact on Human Health; Michael J. Van Stipdonk and H. M. Skip Kingston, Anthony Macherone presiding
Room 341-342

Two-thirds of global mortality is due to chronic disease with cardiovascular disease and cancers as the major causes. Investigations into the underlying factors for disease through genome-wide association studies and data mining have determined that the genetic heritability for these deaths is about 10%. This suggests that majority of causative factors for chronic human disease is not genetic but rather exposure to external and internal chemical entities and of these; only about 50% have been identified. The human exposome represents the totality of these exposures over individuals' lifetime and is a quantity of critical importance needed to understand their impact on disease. This workshop will define and encourage discussions on the human exposome and strategies for its measurement using multi-omics tools within the exposomics paradigm, with an emphasis on use of the exposomic information in guiding research to identify and validate new biomarkers of exposure and disease.

9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message; Ikumi Kayama, MA Medical & Scientific Illustrator presiding
Room 343-344

Clarity in visual communication is as important to scientific meetings as clarity in writing is to journal articles. Most professors and researchers use PowerPoint to create presentations, but very few have taken a course in presentation design or layout. This workshop will offer PowerPoint design tips and tricks to make your presentation better-looking, easier to understand, and more memorable.

One of the most common misuses of PowerPoint slides are as a reading card or a vehicle for information overload. Some presenters make it more difficult to share their work because of hard-to-read slides/graphs and poor visuals. A professional illustrator and scientific communication specialist will teach simple yet effective ways to improve PowerPoint presentations to help professors, researchers, and students present their work more efficiently with better results.

10. Quantitative Glycomics; Yehia Mechref presiding
Room 345-346

Glycosylation of proteins and lipids is one of the most prevalent posttranslational modification with various biological attributes. The functions of many proteins are modulated by glycosylation while anomalous glycosylation has been associated with various mammalian diseases and biological processes. Therefore, the demands to understand the roles of glycans and to monitor the development and progression of diseases have necessitated the development of reliable quantitative glycomics and glycoproteomics methods. A critical discussion of the state-of-the-art glycomics and glycoproteomics methods will be presented at this workshop. Application of these methods to understanding diseases and biological processes will be also presented and discussed. Reliable quantitative glycomics and glycoproteomics is facilitated by bioinformatics tools, an overview of which will be presented.



11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS; Nalini Sadagopan, Susan Abbatiello, Dawn Dufield presiding
Room 347-348

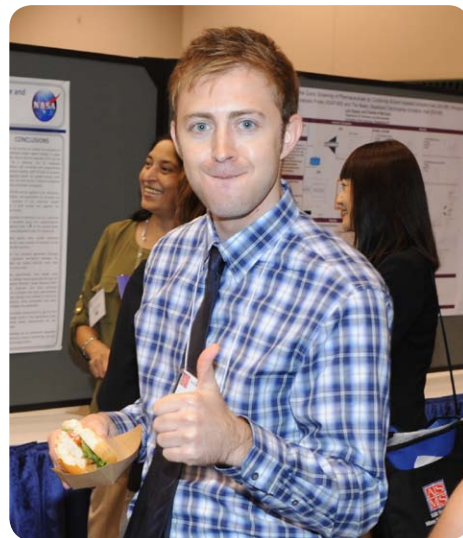
With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS (organized by Flavor Fragrance and Foodstuff Interest Group);
Marc Engel and Timothy Croley presiding
Room 349-350

In the past 10 years there have been many developments in the instrumentation for the analysis of small molecules. With the evolution of GC QQQ and GC HRMS instrumentation, the confidence of quantification and identification of both constituents and contaminants found in flavors and fragrance agents and foodstuffs has increased significantly. After a few brief presentations we will discuss how we can use this instrumentation to improve our analyses.

13. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History; Mehdi Moini, presiding
Room 327

The purpose of this workshop is to discuss the application of mass spectrometry (MS) to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to the application of MS to art and natural history specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of proteinaceous and organic specimens such as silk and wool textiles, leather and animal guts objects, bone and tissues, ink, paper, paint, coatings, binders, and wood. 2) Analysis of the fundamental factors that cause degradation and aging of natural history and art objects; identification of their deterioration markers, using degradation markers as clocks for dating objects, and studying environmental factors that affect deterioration. 3) Application of MS to paleo-organic matter such as fossilomics, amino acid racemization, and ancient DNA. 4) Forensic archeology. 5) Determination of the authenticity of art objects. 6) To be determined.



5:00 - 6:30 PM, SUNDAY
TUTORIAL SESSION
Jenny Brodbelt (University of Texas), presiding
Exhibit Hall AB



5:00 - 5:45 pm
Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know But Were Afraid to Ask

Lucinda Cohen
Merck Research Laboratories



5:45 - 6:30 pm
Imaging Mass Spectrometry

Ron M.A. Heeren
FOM-AMOLF

6:45 - 7:45 PM, SUNDAY
CONFERENCE OPENING
Jenny Brodbelt (University of Texas), presiding
Exhibit Hall AB

Welcome, Jenny Brodbelt
ASMS Vice President for Programs



The James Webb Space Telescope: From First Light to the Search for Earth 2.0

Jason Kalirai
Telescope Science Institute

7:45 - 9:00 PM, SUNDAY
WELCOME RECEPTION
Poster/Exhibit Hall
Conference name badge is required.

8:30 - 10:30 AM, MONDAY MORNING
EMERGING ENVIRONMENTAL CONTAMINANTS
Matthew Crowe (Dow Chemical), presiding
Exhibit Hall AB

MOA am 08:30 **Environmental Petroleomics: Characterization of 10⁵ Biotic and Abiotic Petroleum Transformation Products 4-Years after the Deepwater Horizon Disaster**; Ryan P. Rodgers^{1,4}; Brian M. Ruddy³; Vladislav V. Lobodin^{2,4}; Amy M. McKenna⁴; Huan Chen⁴; David C. Podgorski^{2,4}; Steven M. Rowland¹; Jie Lu^{2,4}; Yuri E. Corilo^{2,4}; Alan G. Marshall^{1,4}; ¹FSU Department of Chemistry and Biochemistry, Tallahassee, FL; ²Future Fuels Institute, Tallahassee, FL; ³Taxon Biosciences Inc., Tiburon, CA; ⁴National High Magnetic Field Laboratory, Tallahassee, FL

MOA am 08:50 **Subtractive Proteomics Reveals Novel Enzymes Induced in Rare Caffeine-Degrading Microorganisms**; Chi Li Yu¹; Ryan Summers²; Yalan Li¹; Sujit Mohanty²; Mani Subramanian³; Marshall Pope¹; ¹Proteomics Facility, Univ. of Iowa, Iowa City, IA; ²Dept. of Chemical and Biochemical Engineering, Iowa City, IA; ³CTR Biocatalysis & Bioprocessing, Univ. of Iowa, Iowa City, IA

MOA am 09:10 **Silicon is a Nearly Ubiquitous Component of Ambient Nanoparticles**; Bryan Bzdek; Ross Pennington; Andrew Horan; Christopher Zordan; Murray Johnston; *University of Delaware, Newark, DE*

MOA am 09:30 **Identification of Environmental Metabolites using Combined High Resolution UPLC- QqTOF and Ultra High Resolution NanoLC-QqITOT Based Approaches**; Jeffrey Gilbert; Jesse Balcer; Yelena Adelfinskaya; Suresh Annangudi; David McCaskill; Pete Johnson; Gerrit Deboer; Mike Hastings; *Dow AgroSciences, Indianapolis, IN*

MOA am 09:50 **Terminal and Internal Alkyne Functionalities in Asphaltenes**; James Riedeman¹; Xingyu Shen¹; Huaming Sheng¹; David Borton²; Matthew Hurt³; Hilikka Kenttämää¹; ¹Purdue University, West Lafayette, IN; ²LECO, St Joseph, MI; ³Chevron, Richmond, CA

MOA am 10:10 **Detection of Water-Borne 4-Methylcyclohexanemethanol (MCHM) via Purge & Trap and Transportable, On-Site GC/MS**; Phil Tackett; Cynthia Liu; Mitch Wells; Dennis Barket; *FLIR Systems, Inc., West Lafayette, IN*

INSTRUMENTATION: NEW DEVELOPMENTS IN HIGH RESOLUTION AND MASS ACCURACY IN HONOR OF ALAN MARSHALL'S 70th BIRTHDAY

Patrick Limbach (University of Cincinnati), presiding
Room 307-308

MOB am 08:30 **Precision Mass Spectrometry on Short-lived Nuclides: New Methods and Results**; Lutz Schweikhard¹; for the SHIPTRAP collaboration²; and the ISOLTRAP collaboration³; ¹University of Greifswald, Greifswald, Germany; ²GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany; ³ISOLDE/CERN, Geneva, Switzerland



MOB am 08:50 **Further Characterization and Applications of Dynamically Harmonized FT ICR Cell**; [Eugene Nikolaev](#)^{1,2}; Gleb Vladimirov¹; Oleg Kharybin³; Matthias Witt⁴; Jochen Friedrich⁴; Roland Jertz⁴; Goekhan Baykut⁴; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russia; ²Emanuel Institute of Biochemical Physics, RAS, Moscow, Russia; ³Orekhovich Institute of Biomedical Chemistry, RAMS, Moscow, Russia; ⁴Bruker Daltonik GmbH, Bremen, Germany

MOB am 09:10 **Pushing the Limits: Using Isotopic Fine Structure Mass Spectrometry to Assist the Understanding of ¹⁷O labelled Peptides in NMR**; [Juan Wei](#)¹; Oleg Antzutkin^{1,2}; Mark Barrow¹; Ray Dupree¹; Steven Brown¹; Peter B. O'connor¹; ¹University of Warwick, Coventry, UK; ²Luleå University of Technology, Luleå, Sweden

MOB am 09:30 **Unexplored Reserves of Resolution in Fourier Transform Mass Spectrometry**; [Anton N. Kozhinov](#); Konstantin O. Nagornov; Daniel Ayoub; Yury O. Tsybin; *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

MOB am 09:50 **High-Field FTICR MS for Imaging Applications: Combining Ultra-High Resolving Power and Mass Accuracy with High Spatial Resolution and Throughput**; [Jeffrey Spraggins](#); Raf Van De Plas; Junhai Yang; Richard Caprioli; *Vanderbilt University, Nashville, TN*

MOB am 10:10 **Development of an FT-ICR Mass Spectrometer in Preparation for 21 Tesla**; [Nathan Kaiser](#)¹; Chad Weisbrod¹; John Quinn¹; Greg T. Blakney¹; Steve Beu²; Tong Chen¹; Christopher L. Hendrickson¹; Alan G. Marshall^{1,3}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²S C Beu Consulting, Austin, TX; ³Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL

**8:30 – 10:30 AM, MONDAY MORNING
NUCLEIC ACIDS**

**Kathrin Breuker (University of Innsbruck), presiding
Room 309-310**

MOC am 08:30 **Single-Molecule Force Spectroscopy and MS Studies of the Determinants of Duplex Stability**; Papa Nii Asare Okai; William Stephenson; Alan Chen; Pan Li; [Daniele Fabris](#); *The RNA Institute, University at Albany, Albany, NY*

MOC am 08:50 **The Effects of Modifications on Glycosidic Bond Stability of Protonated and Sodium Cationized Nucleosides**; [Mary T. Rodgers](#); Yanlong Zhu; *Wayne State University, Detroit, MI*

MOC am 09:10 **LC-MS/MS for the Sensitive Detection of β -Glucosyl-hydroxymethyluracil (Base J) in Genomic DNA of *Trypanosoma brucei***; [Shuo Liu](#)¹; Robert Sabatini²; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA; ²University of Georgia, Athens, Georgia

MOC am 09:30 **Electrospray Mass Spectrometry of Telomeric DNA G-quadruplexes in Potassium**; Adrien Marchand^{1,2}; [Valérie Gabelica](#)^{1,2}; ¹Inserm, U869 ARNA, Bordeaux, France; ²Université de Bordeaux, IECB, Pessac, France

MOC am 09:50 **Fluorescence Measurements of DNA-dye Complexes in the Gas Phase**; [Stephen Sciuto](#)¹; Rebecca A. Jockusch²; ¹The University of Toronto, Toronto, Canada; ²University of Toronto, Toronto, ON

MOC am 10:10 **Conformational Dynamics of DNA G-Quadruplex in Solution Studied by Kinetic Capillary Electrophoresis Coupled On-line with Mass Spectrometry**; Gleb Mironov; Victor Okhonin; Nasrin Khan; [Maxim Berezovski](#); *University of Ottawa, Ottawa, Canada*

**8:30 – 10:30 AM, MONDAY MORNING
FUNDAMENTALS: REACTIONS, DYNAMICS AND THEORY OF
GAS PHASE IONS**

**John Poutsma (College of William and Mary), presiding
Room 314-317**

MOD am 08:30 **Is It a Barrier or Endothermic? The Interesting Cases of Sm⁺ Oxidation by O₂, CO₂, NO, and CO**; Richard Cox¹; Shaun Ard²; Joshua Melko²; Nicholas Shuman²; Al Viggiano²; Ryan Johnson³; Hua Guo³; [Peter Armentrout](#)¹; ¹University of Utah, Salt Lake City, UT; ²Air Force Research Laboratory, Mesa, AZ; ³University of New Mexico, Albuquerque, NM

MOD am 08:50 **Heterometallic Coinage Metal Clusters – Synthesis and Gas-Phase Reactivity**; [George N. Khairallah](#)¹; Richard A. J. O'Hair²; ¹Bio21 Inst, Uni of Melbourne, Melbourne, Australia; ²University of Melbourne, Victoria, Australia

MOD am 09:10 **Exploring Electron and Proton Transfer Timescales in the Gas Phase with Multiscale Pump-Probe Action Spectroscopy Experiments**; [Luke MacAleese](#)¹; Sylvain Hermelin²; Luigi Bonacina²; Rodolphe Antoine¹; Jean-Pierre Wolf²; Philippe Dugourd¹; ¹ILM-UMR5306 Université Lyon 1 - CNRS, Villeurbanne, France; ²GAP-Biophotonics, Université de Genève, Genève, Switzerland

MOD am 09:30 **Determining Masses, Separating Mixtures, and Probing Structures of Native-Like Ions using Selected Cation to Anion Proton Transfer (SCAPT) Reactions**; [Kenneth J. Laszlo](#); Matthew F. Bush; *University of Washington, Seattle, WA*

MOD am 09:50 **Charges in Protein Electrospray Ionization: Like or Opposite?**; [Rachel R. Ogorzalek Loo](#); Joseph A. Loo; *UCLA, Los Angeles, CA*

MOD am 10:10 **Structures and Energetics of Alkali Metal-Bound Clusters of 9-Ethylguanine**; Mohammad Azargun; [Travis Fridgen](#); *Memorial University of NL, St. John's, Canada*

**8:30 – 10:30 AM, MONDAY MORNING
ANTIBODIES AND ANTIBODY-DRUG CONJUGATES**
**Beatrix Ueberheide (New York University), presiding
Ballroom I, level 4**

MOE am 08:30 **Middle-down Primary Structure Assessment and PTM-profiling of Monoclonal Antibody by "Size-controlled" Proteolysis and Online Tandem Mass Spectrometry**; [Weihan Wang](#)¹; Lichao Zhang¹; Michelle English¹; Dina Bai¹; Jeffrey Shabanowitz¹; Donald F. Hunt^{1,2}; ¹Department of Chemistry, University of Virginia, Charlottesville, VA; ²Department of Pathology, University of Virginia, Charlottesville, VA

MONDAY MORNING ORAL SESSIONS

MOE am 08:50 **Middle-Down and Extended Bottom-Up Mass Spectrometry for In-Depth and Rapid Characterization of Immunoglobulins and Their Mixtures**; Daniel Ayoub¹; Luca Fornelli¹; Kristina Srzentic¹; Unige Laskay¹; Alain Beck²; Yury O. Tsybin¹; ¹*Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*; ²*Centre d'Immunologie Pierre Fabre, Saint Julien-en-Genevois, France*

MOE am 09:10 **Informatics for mAb Analysis from Top to Bottom**; Chris Becker¹; Wilfred Tang¹; Yong Kil¹; Marshall Bern¹; John Schiel²; Lisa Kilpatrick²; Trina Formolo²; ¹*Protein Metrics Inc., San Carlos, CA*; ²*National Institute of Standards and Technology, Gaithersburg, MD*

MOE am 09:30 **An Optimized MS-based Pipeline for Producing Repertoires of Recombinant High Affinity Nanobodies**; Yinyin Li¹; Peter Fridy¹; Sarah Keegan²; Mary Thompson¹; Ilona Nudelman¹; David Fenyó²; Michael Rout¹; Brian Chait¹; ¹*The Rockefeller University, New York, NY*; ²*New York University, New York, NY*

MOE am 09:50 **Native MS and IM-MS for Antibody Drug Conjugate Characterization**; François Debaene¹; Amandine Boeuf²; Elsa Wagner-Rousset²; Nathalie Corvaia²; Alain Van Dorsselaer¹; Alain BECK²; Sarah Cianferani¹; ¹*LSMBO - IPHC, Strasbourg, France*; ²*CIPF, Saint Julien en Genevois, France*

MOE am 10:10 **Mass Spectrometry-Based Proteomics in the Development of Antibody Drug Conjugates for Cancer Treatment**; Jeremy Myers; Bingwen Lu; Kim Arndt; *Oncology Research, Pfizer WRD, Pearl River, New York*

8:30 – 10:30 AM, MONDAY MORNING H/D EXCHANGE: NEW DEVELOPMENTS IN TECHNOLOGY Kasper Rand (University of Copenhagen), presiding Ballroom II, level 4

MOF am 08:30 **HDsite: Hydrogen/deuterium Exchange by MS at Amino Acid Resolution**; Zhong-yuan Kan; Wenbing Hu; Benjamin Walters; Leland Mayne; Walter Englander; *University of Pennsylvania, Philadelphia, PA*

MOF am 08:50 **Model-Free Analysis of Millisecond H/D Exchange Reveals Residual Helicity in ACTR, an Intrinsically Disordered Protein**; Theodore Keppel^{1,2}; David Weis¹; ¹*University of Kansas, Lawrence, KS*; ²*Washington University School of Medicine, St. Louis, MO*

MOF am 09:10 **Targeted and Data-Independent Acquisition of Hydrogen/Deuterium Exchange using ETD**; Vladimir Sarpe; David Schriemer; *University of Calgary, Calgary, Canada*

MOF am 09:30 **Conformational Changes in Peripheral Membrane Proteins using Langmuir Monolayers and Hydrogen-Deuterium Exchange Mass Spectrometry**; Gregory F. Pirrone¹; Michael S. Kent²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*Sandia National Laboratories, Albuquerque, NM*

MOF am 09:50 **Characterizing Protein Oligomer Structure and Dissociation Kinetics by Hydrogen/Deuterium Exchange Mass Spectrometry**; Zhe Zhang; Richard Vachet; *University of Massachusetts, Amherst, MA*

MOF am 10:10 **Strategies for Minimizing Spurious In-Source CID for Peptides during ESI-MS**; Siavash Vahidi; Lars Konermann; *Univ. of Western Ontario, London, ON*

8:30 – 10:30 AM, MONDAY MORNING INFORMATICS: PROTEIN IDENTIFICATION David Tabb (Vanderbilt University), presiding Ballroom III, level 4

MOG am 08:30 **Use of Personalized Sequence Databases for Peptide MS/MS Spectrum Matching in the Proteogenomic Analysis of 105 TCGA Breast Tumors**; Karl R. Clauser¹; David Fenyó²; Kelly V. Ruggles²; Philipp Mertins¹; Jana W. Qiao¹; D. R. Mani¹; Michael A. Gillette¹; Sherri R. Davies³; Christopher Maher³; Li Ding³; Matthew J. Ellis³; Steven A. Carr¹; ¹*Broad Institute of MIT and Harvard, Cambridge, MA*; ²*NYU Langone Medical Center, New York, NY*; ³*Washington University, St. Louis, MO*

MOG am 08:50 **Approaching the "Perfect" Database: Single-Molecule, Full-Length Transcript Sequencing to Create Sample-Specific, Full-Length Protein Databases**; Gloria M. Sheynkman; Mark Scalf; Michael R. Shortreed; Brian L. Frey; Anthony J. Cesnik; Lloyd M. Smith; *University of Wisconsin, Madison, WI*

MOG am 09:10 **Novel Galaxy Workflows Combining RNA-seq and Proteomic MS/MS Reveal New Insights into Non-Model Organisms**; Jun Fan¹; Vanessa Evans²; Gary Barker²; Kate Heesom²; Shyamasree Saha¹; David Matthews²; Conrad Bessant¹; ¹*Queen Mary University of London, London, UK*; ²*University of Bristol, Bristol, UK*

MOG am 09:30 **Blind Spectral Alignment with Adaptive Penalties**; Laurence E. Bernstein; Nuno Bandeira; *Univeristy of California, San Diego, La Jolla, CA*

MOG am 09:50 **Pecan: Peptide Identification Directly from Data-Independent Acquisition (DIA) MS/MS Data**; Ying Sonia Ting¹; Jarrett Egerton¹; Brendan Maclean¹; Sangtae Kim²; Samuel H. Payne²; William Stafford Noble¹; Michael J. Maccoss¹; ¹*University of Washington, Seattle, WA*; ²*Pacific Northwest National Laboratory, Richland, WA*

MOG am 10:10 **Doubling Peptide Identification Efficiency in Complex Shotgun Proteomics by Deconvolution and Identification of Multiple Precursors in MS/MS**; Bo Zhang; Mohammad Pirmoradian; Alexey Chernobrovkin; Roman Zubarev; *Karolinska Institutet, Stockholm, Sweden*

8:30 – 10:30 AM, MONDAY MORNING PTMS: ADVANCES IN ISOLATION, ENRICHMENT, DERIVATIZATION AND SEPARATION Jen Grant (University of Wisconsin-Stout), presiding Ballroom IV, level 4

MOH am 08:30 **A Multi-Functionalized Chemical Reagent Capable of Both Gel-Based Detection of Phosphoproteins and Enrichment of Phosphopeptides for Mass Spectrometric Analysis**; Linna Wang; Li Pan; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*

MOH am 08:50 **Characterization of Lipid Modifications on Regulator of G Protein Signaling 4 (RGS4) from Sf9 Cells by Mass Spectrometry**; Yuhuan Ji; Minjing Liu; Markus M. Bachschmid; Catherine E.

- Costello; Cheng Lin; *Boston University School of Medicine, Boston, MA*
- MOH am 09:10 **A Site-Specific Strategy for Localization of D-Amino Acids in Bioactive Peptides**; Chenxi Jia; Qing Yu; Christopher Lietz; Lingjun Li; *University of Wisconsin-Madison, Madison, Wisconsin*
- MOH am 09:30 **Simultaneous Quantitation of S-nitrosylation and Sulfenation Changes in Escherichia coli under Mild Oxidative Stress**; Katarzyna Wojdyla; James Williamson; Peter Roepstorff; Adelina Rogowska-Wrzesinska; *University of Southern Denmark, Odense, Denmark*
- MOH am 09:50 **Protein S-Nitrosylation: Novel Detection, Redox Regulation and Stoichiometry**; Jaimeen Majmudar; Brent Martin; *University of Michigan, Ann Arbor, Michigan*

- MOH am 10:10 **New Methodology for the Enrichment and Characterization of O-GlcNAcylated Peptides**; Stacy Malaker¹; Sarah Penny²; Dina Bai¹; Weihan Wang¹; Mark Cobbold²; Jeffrey Shabanowitz¹; Donald Hunt¹; ¹*University of Virginia, Charlottesville, Virginia*; ²*University of Birmingham, Birmingham, UK*

**10:30 AM – 2:30 PM, MONDAY
MONDAY POSTER SESSION**
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm
12:00 – 1:00 pm
Undergraduate Students
Meet the Experts at tables reserved for you.

MONDAY AFTERNOON ORAL SESSIONS

**2:30 – 4:30 PM, MONDAY AFTERNOON
ANALYSIS OF POLYMER- AND PACKAGING-RELATED
CONTAMINANTS AND DEGRADANTS IN
CONSUMER PRODUCTS**

Avinash Dalmia (PerkinElmer), presiding
Exhibit Hall AB

- MOA pm 2:30 **Top-Down Mass Spectrometry of Hybrid Materials with Hydrophobic Peptide and Hydrophilic Polymer Blocks**; Chrys Wesdemiotis¹; Ahlam Alalwiat¹; Sarah E. Grieshaber²; Bradford A. Paik²; Xinqiao Jia²; ¹*The University of Akron, Akron, OH*; ²*University of Delaware, Newark, DE*
- MOA pm 2:50 **An Application of Mass Spectrometry for the Detection of Chemical Markers for Product Traceability**; Evan Parker; Carlito Lebrilla; *UC Davis, Davis, CA*
- MOA pm 3:10 **Innovative Approaches for Complex Polymer Analysis with the Combination of DART-MS, Thermal Control and a Search Algorithm for Chaotic Spectra**; Kazumasa Kinoshita²; Yuki Kudou¹; Kazuyuki Takama¹; Haruo Shimada³; Yuka Noritake³; Yasuo Shida¹; ¹*Bio Chromato, Inc, Fujisawa, Japan*; ²*DirectAnalysis, Inc, Fujisawa, Japan*; ³*Shiseido Research Center, Yokohama, Japan*
- MOA pm 3:30 **MALDI-TOF/TOF CID Study of Polycarbodiimide Branching Reactions**; Anthony P. Gies; William Heath; *Dow Chemical Company, Freeport, TX*
- MOA pm 3:50 **Matrix Segregation as a Major Cause for Sample Inhomogeneity using the Dried Droplet Sample Preparation Method for MALDI-MSI**; Steffen M. Weidner¹; Stefan Johannes Gabriel¹; Clemens Schwarzingger²; Ulrich Panne¹; ¹*Fed. Inst. f. Mat. Research, Berlin, Germany*; ²*Johannes Kepler University, Linz, At*
- MOA pm 4:10 **Utilization of GC-TOFMS and GC-High Resolution-TOFMS for Characterization of Contaminants and Degradation Products in Consumer Product Packaging Materials**; Ray Marsili¹; Joe Binkley²; ¹*Marsili Consulting Group, Rockford, IL*; ²*LECO Corporation, St. Joseph, MI*

**2:30 – 4:30 PM, MONDAY AFTERNOON
INSTRUMENTATION: MINI/PORTABLE/FIELDABLE
MASS SPECTROMETRY**

Christopher Gill (Vancouver Island University), presiding
Room 307-308

- MOB pm 2:30 **Systematic Testing and Optimization of Subsystems for Development of a Handheld MS**; Mitch Wells; Brent Rardin; Kevin Rosenbaum; Leonard Rorrer; Adam Keil; Dennis Barket; Gary Gentry; *FLIR Systems, West Lafayette, IN*
- MOB pm 2:50 **Development of a Synchronized Discharge Ionization Probe for Direct Analysis of Non-volatile Chemicals on Surfaces Using Handheld Mass Spectrometers**; Xiao Wang; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- MOB pm 3:10 **Handheld Mass Spectrometry Enabled by Ultrahigh Pressure Operation using Air Buffer Gas**; Kevin Schultze; Kenion Blakeman; J. Michael Ramsey; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MOB pm 3:30 **A Loeb-Eiber Mass Filter for Miniature Mass Spectrometry Applications**; William D. Hoffmann; Feng Jin; Glen P. Jackson; *West Virginia University, Morgantown, WV*
- MOB pm 3:50 **Mobile Autonomous Underwater Mass Spec and Sampler System – Opening up the Entire Underwater Chemical Space**; David Fries¹; Geran Barton¹; David Millie²; Robert Ulrich³; John Paul³; ¹*USF, Tampa, Florida*; ²*Michigan Technological University, Ann Harbor, MI*; ³*USF, St. Petersburg, FL*
- MOB pm 4:10 **Utilizing a Novel Compact Mass Spectrometer (CMS) for the Detection and Quantification of Chemical Compounds Related to Cannabis**; Daniel Eikel¹; Simon J. Prosser²; ¹*Advion Inc., Ithaca, NY*; ²*Advion, Inc., Ithaca, NY*

2:30 – 4:30 PM, MONDAY AFTERNOON
ION MOBILITY STRUCTURES
IN HONOR OF MIKE BOWERS' 75TH BIRTHDAY
Gert Von Helden (Fritz-Haber University), presiding
Room 309-310

- MOC pm 2:30 **Are Disulfide Bridges Opened by ETD ?**; Emeline Hanozin; Denis Morsa; Philippe Massonnet; Loic Quinton; [Edwin De Pauw](#); *Mass spectrometry Laboratory, University of Liege, Liege, Belgium*
- MOC pm 2:50 **Substance P from Solution to the Gas Phase: Factors that Stabilize Kinetically Trapped Conformations**; [Kyle L. Fort](#)¹; Joshua A. Silveira¹; Kelly A. Servage¹; Nicholas A. Pierson²; David E. Clemmer²; David H. Russell¹; ¹*Texas A&M University, College Station, TX*; ²*Indiana University Bloomington, Bloomington, IN*
- MOC pm 3:10 **Utilizing High Throughput IMS-MS Measurements to Analyze Small Molecules and Their Noncovalent Interactions with Macromolecular Complexes**; [Erin Baker](#)¹; Ryan Kelly¹; Alex Apffel²; Kristin Burnum-Johnson¹; Young-Mo Kim¹; Yehia Ibrahim¹; Daniel Orton¹; Kevin Crowell¹; Matthew Monroe¹; Thomas Metz¹; Ruwan Kurulugama²; Alex Mordehai²; Ed Darland²; George Stafford²; Gordon Anderson¹; Richard Smith¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Agilent Technologies, Santa Clara, CA*
- MOC pm 3:30 **Supercharging of Native Protein Complexes: Effects of Polarity and Evidence for Multiple Mechanisms**; [Samuel J. Allen](#); Christiane N. Stachl; Matthew F. Bush; *University of Washington, Seattle, WA*
- MOC pm 3:50 **Ion Mobility and Solution Studies Show Specific Competitive Binding of Homo- and Heteromultimer Receptor:Protein:Carbohydrate Binding**; [Julie A. Leary](#); Youjin Seo; *UC Davis, Davis, CA*
- MOC pm 4:10 **Projected Superposition Approximation: A Novel Parameter Set for Prediction of Cross Sections in Nitrogen as a Drift Gas**; [Christian Bleiholder](#)¹; Thomas Wyttenbach²; Michael T. Bowers²; ¹*Florida State University, Tallahassee, FL*; ²*University of California, Santa Barbara, CA*

2:30 – 4:30 PM, MONDAY AFTERNOON
PHOTOIONIZATION
Helene Cardasis (Thermo Scientific), presiding
Room 314-317

- MOD pm 2:30 **Evaluation of the Optimization Space for Atmospheric Pressure Photoionization (APPI)**; [Andreas Fredenhagen](#); Jürgen Kühnöl; *Novartis, Basel, Switzerland*
- MOD pm 2:50 **Highly Time-Resolved Mapping of Combustion Product-Concentrations in Dynamic Solid-Fuel Combustion Processes by Photoionisation Mass Spectrometry: Looking into a Burning Cigarette**; [Ralf Zimmermann](#)¹; Romy Hertz-Schuenemann¹; Sven Ehlert¹; Kevin PCAadam²; Steven Coburn²; Chuan Liu²; Thorsten Streibel¹; ¹*University of Rostock, Rostock, Germany*; ²*GR&D, BAT Ltd., Southampton, UK*
- MOD pm 3:10 **Investigating the Ionization of Sulfur-Containing Compounds within Petroleum using Atmospheric Pressure Photoionization Fourier Transform Ion**

Cyclotron Resonance Mass Spectrometry; Holly Chan; [Mark Barrow](#); *University of Warwick, Coventry, UK*

- MOD pm 3:30 **Fluorophore-Assisted Laser Desorption/Ionization Mass Spectrometry (FALDI-MS) of biomolecules**; [Dragan Isailovic](#); Raymond West; Eric Findsen; *The University of Toledo, Toledo, OH*
- MOD pm 3:50 **Laser Desorption VUV Lamp Ionization for Quadrupole Ion Trap Mass Spectrometry**; [Qinghao Wu](#); Richard Zare; *Stanford University, Stanford, CA*
- MOD pm 4:10 **Analytical Performance of a Novel, Dopant-Free GC-APPI Source with Femtogram-Level Sensitivity for Quadrupole-Orbitrap GC/MS**; [Amelia C. Peterson](#)¹; Hendrik Kersten²; Dirk Krumwiede¹; Scott Quarmby³; Kyle D'Silva¹; Kai Kroll²; Kirsten Haberer²; Maciej Bromirski¹; Alexander Makarov¹; Thorsten Benter²; ¹*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ²*University of Wuppertal, Wuppertal, Germany*; ³*Thermo Fisher Scientific, Austin, TX*

2:30 – 4:30 PM, MONDAY AFTERNOON
CHARACTERIZATION OF BIOLOGICALS AND BIOSIMILARS
James Madsen (Momena Pharmaceuticals), presiding
Ballroom I, level 4

- MOE pm 2:30 **Sequence Variant Analysis with Increased Specificity and Meaningful Confidences**; [Sean L. Seymour](#); Ignat V. Shilov; Joe Durant; Bret Pehrson; Eric Johansen; *AB SCIEX, Redwood City, CA*
- MOE pm 2:50 **Size-Based Enrichment and 1D Proteomics of Low ppm Levels of Host Cell Proteins in High-Concentration Therapeutic Antibodies**; Gang Xiao; Da Ren; [Pavel Bondarenko](#); *Amgen, Inc., Thousand Oaks, CA*
- MOE pm 3:10 **Interleukin-23 Binding to Adnectin: An Approach to Correlating Molecular Structure with Hydrogen/Deuterium Exchange Mass Spectrometry**; [Roxana E. Jacob](#)¹; Guodong Chen²; Stanley R. Krystek²; Hui Wei²; Richard Huang²; Li Tao²; Zheng Lin²; Paul E. Morin²; Michael L. Doyle²; Adrienne A. Tymiak²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*Bristol-Myers Squibb, Princeton, NJ*
- MOE pm 3:30 **New Workflows for Identification and Profiling of Disulfide Bonds in Biopharmaceuticals**; Jan Wiesner; Antje Kozicki; Anja Resemann; Rainer Paape; Lars Vorwerg; Kristina Marx; Andrea Kiehne; Ralf Hartmer; Carsten Baessmann; Detlev Suckau; [Wolfgang Jabs](#); *Bruker Daltonik GmbH, Bremen, Germany*
- MOE pm 3:50 **System Suitability Metrics for Analysis of Protein Therapeutics by LC-MS**; [Mowei Zhou](#); Ashley Gucinski; Michael Boyne; *U.S. FDA, Division of Pharmaceutical Analysis, St Louis, MO*
- MOE pm 4:10 **Biopharmaceutical Characterization: Evaluation of the NIST Monoclonal Antibody Reference Material.**; [John Schiel](#)¹; Meiyao Wang¹; Trina Formolo¹; Lisa Kilpatrick¹; Mark Lowenthal¹; Henning Stockmann²; Karen Phinney¹; Justin Prien³; Darryl Davis⁴; Oleg Borisov³; ¹*NIST, Gaithersburg, MD*; ²*NIBRT, Dublin, Ireland*; ³*Novavax, Gaithersburg, MD*; ⁴*Janssen, Malvern, PA*; ⁵*Amgen, West Greenwich, RI*



**2:30 – 4:30 PM, MONDAY AFTERNOON
QUANTITATIVE ANALYSIS IN
DRUG DISCOVERY AND DEVELOPMENT**
Brian Furmanski (GlaxoSmithKline), presiding
Ballroom II, level 4

MOF pm 2:30 **Digestion of Some Model Proteins for Therapeutic Proteins in Blood Plasma with Thermolysin and Quantification of the Peptides by LC/LC-MS/MS;** Aljona Saleh; *Stockholm university, Analytical Chemistry, Stockholm, Sweden*

MOF pm 2:50 **High-Throughput, Dual-Stream UHPLC/MS/MS Bioanalysis and Data-Deconvolution for Rapid Drug Discovery Applications;** Brendon Kapinos¹; John Janiszewski¹; Mary Piotrowski¹; Wayne Lootsma²; Steve Ainley²; Nick Levitt³; ¹*Pfizer Inc., Groton, CT*; ²*Sound Analytics, Niantic, CT*; ³*Two Center Technologies, Cambridge, MA*

MOF pm 3:10 **Single Cell Drug Discovery;** Sachiko Date¹; Hajime Mizuno¹; Tsuyoshi Esaki¹; Ai Fujita¹; Tsutomu Masujima¹; Haruo Iwabuchi²; Makoto Takei²; Hideo Takakusa²; Takashi Izumi²; Setsuko Fujita³; Shuichi Matsuda³; Motohiko Morihara³; Kiyoko Bando⁴; Jiro Deguchi⁴; Yasunori Fukuda⁵; Naoki Tarui⁵; ¹*Quantitative Biology Center (QBiC), RIKEN, Suita, Osaka, Japan*; ²*Daiichi Sankyo Co. Ltd., Shinagawa, Tokyo, JP*; ³*Ono Pharmaceutical Co., Ltd., Shimamoto, Osaka, JP*; ⁴*Dainippon Sumitomo Pharma Co. Ltd., Osaka, JP*; ⁵*Takeda Pharmaceutical Co., Ltd, Fujisawa, Kanagawa, JP*

MOF pm 3:30 **A Novel Selective Peptide Derivatization Strategy for Sensitivity Enhancement for the LC-MS/MS Bioanalysis of Protein Therapeutics in Serum;** Long Yuan¹; Anna Mai²; Anne-Françoise Aubry¹; Mark Arnold¹; Qin Ji¹; ¹*Bristol-Myers Squibb, Princeton, NJ*; ²*Columbia University, New York, NY*

MOF pm 3:50 **Label-Free Quantification of GeLC-MALDI Data with a Novel Software Reveals Pancreatic Ductal Adenocarcinoma Subtype-Specific Protein Signatures;** Wiebke Nadler^{1,3}; Alexander Kerner^{1,3}; Sabrina Hanke^{1,3}; Christoph Roesli^{1,2}; ¹*Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany*; ²*Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany*; ³*Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany*

MOF pm 4:10 **Total Plasma 3-chloro-tyrosine and Methionine Sulfoxide are Biomarkers of Oxidative Stress Events in Humans;** Matthew Blatnik¹; Rick Steenwyk¹; Paul Huang²; Buckbinder Leonard³; ¹*Pfizer Inc., Groton, CT*; ²*Massachusetts General Hospital and Harvard Medical, Boston, MA*; ³*Pfizer Inc., Cambridge, MA*

**2:30 – 4:30 PM, MONDAY AFTERNOON
INFORMATICS: PROTEIN QUANTIFICATION**
Nathan Yates (University of Pittsburgh), presiding
Ballroom III, level 4

MOG pm 2:30 **Proteome-Wide Analysis of Diversity Outbred Mouse Liver Protein Expression in Relation to Genetic and Environmental Variability;** Joel M. Chick¹; Steven Ciciotte²; Steven C. Munger²; Daniel M. Gatti²; Karen L. Svenson²; Gary A. Churchill²; Steven P. Gygi¹; ¹*Harvard medical school, Boston, MA*; ²*The Jackson Laboratory, Bar Harbor, MA*

MOG pm 2:50 **Streamlining Sequence Variant and Modification Analysis of Therapeutic Proteins;** Yong Kil¹; Chris Becker¹; Oleg Borisov²; Boyan Zhang³; Michael Kim⁴; Richard Seipert⁴; ¹*Protein Metrics Inc., San Carlos, CA*; ²*Novavax, Inc., Gaithersburg, MD*; ³*Beijing Mabworks Biotech Co., Ltd., Beijing, China*; ⁴*Genentech, South San Francisco, CA*

MOG pm 3:10 **CONSTAND : A Normalization Method for Isobaric Labeled Spectra by Constrained Programming;** Evelyne Maes^{1,2}; Wahyu Hadiwikarta^{1,2}; Inge Mertens¹; Geert Baggerman^{1,3}; Jef Hooyberghs^{1,4}; Dirk Valkenborg^{1,4}; ¹*VITO, Mol, Belgium*; ²*KULeuven, Leuven, Belgium*; ³*UAntwerpen, Antwerpen, Belgium*; ⁴*UHasselt, Hasselt, Belgium*

MOG pm 3:30 **Proteomform Quantitation through the IQ Framework;** Grant Fujimoto; Sangtae Kim; Kevin Crowell; Nikola Tolic; Charles Ansong; Si Wu; Ljiljana Pasa-Tolic; Richard D. Smith; Joshua Adkins; Sam Payne; *Pacific Northwest National Laboratory, Richland, WA*

MOG pm 3:50 **Statistical Elimination of Spectral Features with Large Between-Run Variation Enhances Quantitative Protein-Level Conclusions in Experiments with Data-Independent Spectral Acquisition;** Lin-Yang Cheng¹; Yansheng Liu²; Ching-Yun Chang¹; Hannes Roest²; Ruedi Aebersold^{2,3}; Olga Vitek^{1,4}; ¹*Department of Statistics, Purdue University, West Lafayette, IN*; ²*Department of Biology, ETH, Zurich, Switzerland*; ³*Faculty of Science, University of Zurich, Zurich, Switzerland*; ⁴*Department of Computer Science, Purdue University, West Lafayette, IN*

MOG pm 4:10 **Public Sharing of Complex MS-based Qualitative and Quantitative Proteomic Data Analysis Workflows: Adding Value to big Data Repositories;** Tim Griffin¹; Pratik Jagtap¹; James Johnson²; Trevor Wennblom²; Bart Gottschalk²; Yue Chen¹; ¹*University of Minnesota, Minneapolis, MN*; ²*Minnesota Supercomputing Institute, Minneapolis, MN*

**2:30 – 4:30 PM, MONDAY AFTERNOON
IMAGING: BIOLOGICAL APPLICATIONS**
Richard Perry (University of Illinois), presiding
Ballroom IV, level 4

MOH pm 2:30 **Advanced MALDI Imaging Techniques for the Study of Renal Disease;** Megan M. Gessel¹; Jeffrey Spraggins¹; Raf Van De Plas¹; Dale Abrahamson²; Billy Hudson¹; Richard Caprioli¹; ¹*Vanderbilt University School of Medicine, Nashville, TN*; ²*University of Kansas Medical Center, Kansas City, KS*

MOH pm 2:50 **Chronic Ethanol Consumption Profoundly Disrupts Regional Brain Ceramide-Sphingomyelin Content in a Mouse Model;** Amina S. Woods¹; Aurelie Roux¹; Shelley N Jackson¹; Ludovic Muller¹; J. Albert Schultz²; Joseph R. O'Rourke³; Panayotis K. Thanos³; Nora D Volkow¹; ¹*NIDA-IRP, NIH, Baltimore, MD*; ²*Ionwerks, Inc., Houston, TX*; ³*Stony Brook University, Stony Brook, NY*

MOH pm 3:10 **Spatially Resolved Rapid Evaporative Ionization Mass Spectrometry (REIMS) for Database Population and In-Theatre Classification of Excised Tissues;** Emrys A Jones; Ottmar Golf; Nicole Strittmatter; Abigail Speller; Zoltan Takats; *Imperial College London, London, UK*

MONDAY AFTERNOON AND TUESDAY MORNING ORAL SESSIONS

MOH pm 3:30 **Molecular Signatures and Implications of Focal Cerebral Ischemia Revealed using Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging;** [Ingela Lanekoff](#)^{1,3}; Susan Stevens²; Mary Stenzel-Poore²; Julia Laskin^{1,3}; ¹PNNL, Richland, WA; ²Oregon Health & Science University, Portland, OR; ³Pacific NW National Laboratory, Richland, WA

MOH pm 3:50 **Combining Magnetic Resonance Spectroscopic Imaging and Mass Spectrometric Imaging Reveals Protein Biomarkers of Aggressive Breast Cancer;** [Lu Jiang](#)¹; Kamila Chughtai²; Tiffany Greenwood¹; Zaver Bhujwalla¹; Venu Raman¹; Gert Eijkel²; Ron Heeren²; Kristine Glunde¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD; ²FOM-Institute AMOLF, Amsterdam, The Netherlands

MOH pm 4:10 **3D Molecular Cartography of Humans;** [Amina Bouslimani](#)¹; Carla Porto Da Silva¹; Christopher M Rath¹; Mingxun Wang¹; Guo Yurong¹; Antonio Gonzalez²; Donna Berg-Lyon²; Gail Ackermann²; Gitte Julie Moeller Christensen³; Nakatsuji Teruaki¹; Lingjuan Zhang¹; Andrew Borkowski¹; Michael Meehan¹; Kathleen Dorrestein¹; Richard Gallo¹; Nuno Bandeira¹; Rob Knight²; Theodore Alexandrov⁴; Pieter Dorrestein¹; ¹Univ. of California at San Diego, La Jolla, CA; ²University of Colorado at Boulder, Boulder, CO; ³Aarhus University, Aarhus, Denmark; ⁴University of Bremen, Bremen, Germany

4:45 – 5:30 PM, MONDAY AFTERNOON AWARD LECTURE

**Susan T. Weintraub (Univ. of Texas HSC, San Antonio), presiding
Exhibit Hall AB**



Award for a Distinguished Contribution in Mass Spectrometry

Richard M. Caprioli
Vanderbilt University

5:45 – 7:00 PM, MONDAY AFTERNOON WORKSHOPS

Level 3

Light refreshments, level 3

1. Real World Applications of Photoionization; Room 307-308
2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group); Room 309-310
3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Room 314-317
4. How to Succeed in Pharma without Really Trying; Room 327
5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group); Room 336
6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum & Biofuels Interest Group); Room 337
7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); Room 338
8. ProteomicsDB; Room 339-340
9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Room 341-342
10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry (organized by Lipids and Lipidomics Interest Group); Room 343-344
11. A State of the Union for Biomarker Translation (organized by Clinical Chemistry Interest Group); Room 345-346
12. Antibody Drug Conjugates as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Room 347-348
13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security (organized by Forensics and Homeland Security Interest Group); Room 349-350

**AFTER 8:00 PM, MONDAY EVENING
CORPORATE HOSPITALITY SUITES
Hilton Hotel**

TUESDAY MORNING ORAL SESSIONS

**8:30 – 10:30 AM, TUESDAY MORNING
INTEGRATED QUALITATIVE AND QUANTITATIVE LC-MS FOR
SMALL MOLECULE ANALYSIS**
**Alison Danell (East Carolina University), presiding
Exhibit Hall AB**

TOA am 08:30 **Probing Dynamics of Plant Specialized Metabolism through Stable Isotopic Labeling and Nonselective Collision-Induced Dissociation;** [Zhenzhen Wang](#); A. Daniel Jones; Michigan State University, East Lansing, MI

TOA am 08:50 **Characterizing Chemical Composition of SOM using Graduated Extractions, Deep Fractionation and LCMS to Detect/Quantify a Broad Range of Compounds;** [Kristyn Roscioli](#)¹; Yufeng Shen²; Thomas Fillmore¹; Rui Zhao¹; Nikola Tolic¹; Brian Anderson²; Nancy J Hess¹; Ljiljana Paša-Tolić¹; Errol W Robinson¹; ¹Environmental Molecular Sciences Laboratory, PNNL, Richland, WA; ²Biological Sciences Division, PNNL, Richland, Washington

TOA am 09:10 **Analysis of Enantiomeric Amino Acids in Biological Samples via Capillary Electrophoresis Coupled with Mass Spectrometry;** [Takayuki Kawai](#); Stanislav Rubakhin; Jonathan Sweedler; University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

TOA am 09:30 **Characterization of Alkylpolyglucoside Surfactants with Liquid Chromatography/Mass Spectrometry and Evaporative Light Scattering Detection: Total Characterization without a Reference Standard;** [Matthew Crowe](#); Katherine Davis; Janet Windisch; Dow Chemical Company, Collegeville, PA

TOA am 09:50 **Application of Qualitative and Quantitative Analysis of HRMS to Fast Identification of Major Drug Metabolic Pathways and Drug-Metabolizing Enzymes;** [Qian Ruan](#); Li Ma; Mingshe Zhu; Dept. of Biotransformation, Bristol-Myers Squibb, Princeton, NJ

TOA am 10:10 **Combining Derivatization and SWATH for the Integrated Quantification and Identification of Aldehydes and Ketones in Biological Samples;** David Siegel¹; Anne Meinema¹; Hjalmar Permentier¹; Gerard Hopfgartner²; Rainer Bischoff¹; ¹University of Groningen, Groningen, Netherlands; ²University of Geneva, Geneva, Switzerland

**8:30 – 10:30 AM, TUESDAY MORNING
INSTRUMENTATION AND METHODS: FT, ION TRAPS AND
HYBRID INSTRUMENTS**

**Ryan Danell (Danell Consulting), presiding
Room 307-308**

TOB am 08:30 **Hybrid Electron Transfer/Ultraviolet Photodissociation for Characterization of Intact Proteins;** Joe Cannon; Dustin Holden; Jennifer Brodbelt; University of Texas, Austin, TX

TOB am 08:50 **Absolute Pressure in FTICR/MS Using “CRAFTI” Technique For Measuring Collision Cross Sections;** Chad Jones; David V. Dearden; Brigham Young University, Provo, UT

TOB am 09:10 **A New Method for Isolating Ions in Quadrupole Ion Traps Using an Excitation Waveform Generated by Frequency Modulation and Upconversion;** Ryan T. Hilger; Robert E. Santini; Boone M. Prentice; Scott A. McLuckey; Purdue University, West Lafayette, IN

TOB am 09:30 **Dual-Trap Configuration for High Efficiency Tandem Mass Spectrometry Analysis;** Linfan Li; Xiaoyu Zhou; Zheng Ouyang; Purdue University, West Lafayette, IN

TOB am 09:50 **Lossless Ion Trapping in Structures for Lossless Ion Manipulation (SLIM);** Xinyu Zhang; Sandilya V.B. Garimella; Spencer A. Prost; Ian K. Webb; Randolph V. Norheim; Brian L. LaMarch; Tsung-Chi Chen; Aleksey V. Tolmachev; Gordon A. Anderson; Yehia M. Ibrahim; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA

TOB am 10:10 **Setting New Speed Records for Orbitrap Mass Spectrometry;** Alexander Makarov; Jan-Peter Hauschild; Eduard Denisov; Amelia Peterson; Oliver Lange; Eugen Damoc; Mathias Mueller; Konstantin Ayzikov; Andreas Wieghaus; Markus Kellmann; Thermo Fisher Scientific, Bremen, Germany

**8:30 – 10:30 AM, TUESDAY MORNING
ION MOBILITY: SEPARATIONS**

**Stephen Valentine (West Virginia University), presiding
Room 309-310**

TOC am 08:30 **Progress in the Development of Structures for Extended and Lossless Ion Separations and Manipulations;** Richard D. Smith; Xinyu Zhang; Ian Webb; Tsung-Chi Chen; Sandilya Garimella; Aleksey Tolmachev; Yehia Ibrahim; Gordon Anderson; Erin Baker; PNNL, Richland, WA

TOC am 08:50 **Ion Mobility Spectrometry of Foldamers;** Frédéric Rosu¹; Christian Klein²; Xuesong Li^{3,4}; Victor Maurizot^{3,4}; Ivan Huc^{3,4}; Valérie Gabelica^{4,5}; ¹CNRS UMS 3033, Inserm U001, IECB, Pessac, France; ²Agilent Technologies, Santa Clara, CA; ³CNRS, UMR 5284, CBMN, Pessac, France; ⁴Université de Bordeaux, IECB, Pessac, France; ⁵Inserm, U869 ARNA, Bordeaux, France

TOC am 09:10 **Accuracy in Ion Mobility Spectrometry: Requirements and Results;** Brian Hauck¹; Bill Siems¹; Charles Harden²; Vincent McHugh³; Herbert Hill, Jr.¹; ¹Washington State University, Pullman, WA; ²LEIDOS - US Army ECBC Operations, Gunpowder, MD; ³U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD

TOC am 09:30 **Ion Mobility Mass Spectrometry Differentiates Multiprotein Complex Structures formed in Solution and in Electrospray Droplets;** Linjie Han; Brandon Ruotolo; University of Michigan, Ann Arbor, MI

TOC am 09:50 **Structural Characterization of Methylenedianiline Regioisomers by Ion Mobility-Mass Spectrometry, Tandem Mass Spectrometry, and Computational Strategies;** Sarah M. Stow¹; Jay G. Forsythe¹; Tiffany M. Onifer¹; Hartmut Nefzger²; Nicholas W. Kwiecien³; Jody C. May¹; David M. Hercules¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN; ²Bayer MaterialScience AG, Leverkusen B108, Germany; ³University of Wisconsin, Madison, WI

TOC am 10:10 **IR Spectroscopy of IMS-MS Selected Protein Ions;** Stephan Warnke; Kevin Pagel; Gert von Helden; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

**8:30 – 10:30 AM, TUESDAY MORNING
MACROMOLECULAR COMPLEXES: ACTIVATION AND
DISSOCIATION**

**Brian Bothner (Montana State University), presiding
Room 314-317**

TOD am 08:30 **Multi-Step Sequencing and Confident Identification of Native Protein Complexes with an Orbitrap Mass Spectrometer;** Mikhail Belov^{1,3}; Eugen Damoc³; Eduard Denisov³; Philip Compton²; Neil L. Kelleher²; Alexander Makarov³; ¹Spectrograph LLC, Kennewick, WA; ²Northwestern University, Evanston, IL; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

TOD am 08:50 **Protein Complexes: Breaking Up is Hard to Do (Unless You Have an FTMS);** Huilin Li; Jiang Zhang; Piriya Wongkongkathep; Rachel R. Ogorzalek Loo; Joseph A. Loo; UCLA, Los Angeles, CA

TOD am 09:10 **Surface Induced Dissociation (SID) and Collision Induced Dissociation (CID) Characterization of Human Nucleosomes;** Yun Zhang; Xin Ma; Morgan Bernier; Cecil Howard; Michael Poirier; Jennifer Ottesen; Vicki Wysocki; The Ohio state university, Columbus, OH

TOD am 09:30 **Probing Protein Stability, Unfolding and Dissociation with Variable Temperature Mass Spectrometry and Variable Temperature Ion Mobility Mass Spectrometry;** Kamila Pacholarz¹; Perdita Barran²; ¹University of Edinburgh, Edinburgh, UK; ²University of Manchester, Manchester, UK

TOD am 09:50 **Top-Down Characterization of Non-Covalent Protein Complexes via Ultraviolet Photodissociation Mass Spectrometry;** John O'Brien; Jennifer Brodbelt; University of Texas, Austin, TX

- TOD am 10:10 **Association of the Dual Specificity Phosphatase DUSP12 with Various Messenger Ribonucleoprotein Particles Revealed by Interactome Analysis**; Panayiotis Vacratsis; *University of Windsor, Windsor, Canada*
- 8:30 – 10:30 AM, TUESDAY MORNING
PK/PD ANALYSIS OF BIOLOGICS
John Schiel (NIST), presiding
Ballroom I, level 4**
- TOE am 08:30 **Transitioning to High-Resolution MS for Bioanalytical Study Support: Comparison of High Resolution MS Technologies**; John Kellie; Jonathan Kehler; Matthew Szapacs; *GSK, King Of Prussia, PA*
- TOE am 08:50 **In vivo Quantitation of Endosome-Disruptive Peptides using High-Resolution Mass Spectrometry to Support Pharmacokinetic Studies**; Bao-Jen Shyong; Rob Burke; Rubina Parmar; Elizabeth Mahan; Suzie Yeh; Rena Zhang; Mark Cancilla; *Merck & Co. Inc., West Point Plant, PA*
- TOE am 09:10 **Expanding the Possibilities of LC-MS/MS for the Quantification of (Therapeutic) Proteins in Complex Biological Matrices**; Kees Bronsema^{1,2}; Rainer Bischoff¹; Nico van de Merbel^{1,2}; *¹University of Groningen, Groningen, The Netherlands; ²PRA, Assen, The Netherlands*
- TOE am 09:30 **Applying Acid Dissociation in LC-MS/MS Analysis of A PEGylated Anti-CD28 Domain Antibody in Human Serum**; Chao Gong; Jianing Zeng; Billy Akinsanya; Hao Jiang; Johanna Mora; Shannon Chilewski; Janice Gambardella; Alban Allentoff; Carol Gleason; Anne-Francoise Aubry; Binodh DeSilva; Mark Arnold; *Bristol-Myers Squibb, Princeton, NJ*
- TOE am 09:50 **LC-MS/MS Approaches to Support Clinical Studies of an Extended Half-Life Bioactive Peptide Fused to an Albumin-Binding Domain Antibody**; Chester L. Bowen; Jonathan Kehler; Thomas Mencken; Bonnie Orr; Matthew Szapacs; *GlaxoSmithKline, King Of Prussia, PA*
- TOE am 10:10 **Biodistribution Studies of Transferrin-Based Drug in Animal Models by Inductively Coupled Plasma Mass Spectrometry (ICP-MS)**; Son N. Nguyen; Hanwei Zhao; Shunhai Wang; Cedric Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- 8:30 – 10:30 AM, TUESDAY MORNING
H/D EXCHANGE: BIOLOGICAL APPLICATIONS
Derek Wilson (York University), presiding
Ballroom II, level 4**
- TOF am 08:30 **Setting the Stage: Recent Developments in HDX/MS for Exploring Protein Folding, Structure, Dynamics, and Interactions**; Lars Konermann; *Univ. of Western Ontario, London, Canada*
- TOF am 08:50 **Elucidating the Mechanisms of Antibody Neutralization of HIV Env by H/D Exchange**; Miklos Guttman¹; Jean-Philippe Julien²; Al Cupo³; Rogier Sanders³; Ian Wilson²; John Moore³; Kelly Lee¹; *¹University of Washington, Seattle, WA; ²Scripps Research Institute, La Jolla, CA; ³Weill Medical College of Cornell University, New York, NY*
- TOF am 09:10 **Deubiquitinase-Induced Stabilization of Proteasomal Subunit Rpn1 Revealed by Hydrogen Exchange Mass Spectrometry**; Bradley Stocks¹; Geng Tian²; Suzanne Elsasser²; Daniel Finley²; John R. Engen¹; *¹Northeastern University, Boston, MA; ²Harvard Medical School, Boston, MA*
- TOF am 09:30 **Investigating the Interaction of an IgG₁ Antibody with the Neonatal Fc Receptor by HDX-MS and ETD**; Pernille Foged Jensen¹; Vincent Larraillet²; Maximiliane Hilger²; Kasper D. Rand¹; *¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Pharma Research, Roche Diagnostics GmbH, Penzberg, Germany*
- TOF am 09:50 **HDX Analysis of RGS-Gα and Multimeric Protein Complexes; Use of Isotopic Labeling**; Devrishi Goswami¹; Nicole Brown²; Bruce Pascal¹; Steve Tusky³; Eddy Arnold³; John Hepler²; Patrick Griffin¹; *¹The Scripps Research Institute, Scripps Florida, Jupiter, FL; ²Emory University, Atlanta, Georgia; ³Rutgers University, Piscataway, New Jersey*
- TOF am 10:10 **Implementing H/DX-MS in Therapeutic Protein Formulation Development**; Jun Zhang; Douglas Banks; Michael Treuheit; Gerald Becker; *Amgen, Inc, Seattle, WA*
- 8:30 – 10:30 AM, TUESDAY MORNING
PHOSPHOPROTEOMICS IN DISEASE
Ying Ge (University of Wisconsin), presiding
Ballroom III, level 4**
- TOG am 08:30 **Proteogenomic Analysis of Human Breast Cancer Connects Genetic Alterations to Phosphorylation Networks**; Philipp Mertins¹; Jana Qiao¹; Karl R. Clauser¹; D. R. Mani¹; Michael Gillette¹; Kelly Ruggles²; David Fenyo³; Sherri Davies⁴; Pei Wang⁵; Ping Yan⁶; Chenwei Lin⁶; Sean Wang⁶; Yuzheng Zhang⁶; Michael McLellan⁴; Henry Rodriguez⁷; Reid Townsend⁴; Li Ding⁴; Amanda Paulovich⁶; Matthew Ellis⁴; Steven A. Carr¹; *Clinical Proteomic Tumor Analysis Consortium (CPTAC)⁷; ¹The Broad Institute of MIT and Harvard, Cambridge, MA; ²NYU Langone Medical Center, New York, NY; ³New York University, New York, NY; ⁴Washington University, St. Louis, MO; ⁵Icahn School of Medicine at Mount Sinai, New York, NY; ⁶Fred Hutchinson Cancer Research Center, Seattle, WA; ⁷National Cancer Institute, Bethesda, MD*
- TOG am 08:50 **Identification of Post-translational Modifications of Human Desmoplakins in Regulating Interactions with Intermediate Filaments**; Lichao Zhang¹; Lauren Albrecht²; Kathleen Green^{2,3}; Jeffrey Shabanowitz¹; Donald Hunt^{1,4}; *¹Department of Chemistry, University of Virginia, Charlottesville, VA; ²Department of Pathology, Northwestern University, Chicago, IL; ³Department of Dermatology, Northwestern University, Chicago, IL; ⁴Department of Pathology, University of Virginia, Charlottesville, VA*
- TOG am 09:10 **Quantitative Phosphoproteomic Analysis of the PTEN Signaling Pathway**; Sadiq Zahari; Jacqueline Douglass; Min Sik Kim; Patrick Shaw; Derese Getnet; Ben Park; Xinyan Wu; Akhilesh Pandey; *Johns Hopkins School of Medicine, Baltimore, MD*
- TOG am 09:30 **Phosphoproteome Profiling of Toll-Like Receptor Response to Different Ligand Stimulation in Macrophages; Role of MARCKS Ser163 Phosphorylation**; Virginia Sjoelund; Margery Smelkinson; Iain Fraser; Aleksandra Nita-Lazar; *NIH, Bethesda, MD*

TOG am 09:50 **Multi-Notch MS3-Based 10-Plex TMT Quantification of Human Colorectal Cancer Cells Reveals Distinct Temporal Phosphoproteomic Profiles in Wnt Signaling;** Mark P. Jedrychowski; Ryan Kunz; Robert A. Everley; David P. Nusinow; Leonid Peshkin; Marc W. Kirschner; Steven P. Gygi; *Harvard Medical School, Boston, MA*

TOG am 10:10 **Drug-based Phosphoproteomic Study of Human Insulin Receptor Phosphorylation with Nano-flow UPLC-MS and UPLC-MS/MS;** Jason X. Tang; Zhongping Liao; John Beals; *Eli Lilly & Company, Indianapolis, IN*

8:30 – 10:30 AM, TUESDAY MORNING

IMAGING: PHARMACEUTICALS AND METABOLOMICS

Lingjun Li (University of Wisconsin-Madison), presiding
Ballroom IV, level 4

TOH am 08:30 **Pharmaceutical Mass Spectrometry Imaging: A Cross Platform Approach for Both Targeted and Untargeted Molecular Histology;** Richard Goodwin¹; John Swales¹; Anna Nilsson²; C. Logan Mackay³; Per Andren²; Jennifer Sasaki⁴; Peter Webborn¹; Anshul Gupta⁴; ¹*AstraZeneca, Macclesfield, UK*; ²*Uppsala University, Uppsala, Sweden*; ³*University of Edinburgh, Edinburgh, UK*; ⁴*AstraZeneca, Waltham, MA*

TOH am 08:50 **Mapping HIV Drugs in Tissue using IR-MALDESI MSI Coupled to the Q Exactive with Several Acquisition Modes;** David C. Muddiman¹; Jeremy Barry¹; Guillaume Robichaud¹; Mark Bokhart¹; Corbin Thompson²; Craig Sykes²; Angela Kashuba²; ¹*North Carolina State University, Raleigh, NC*; ²*UNC Chapel Hill, Chapel Hill, NC*

TOH am 09:10 **Multimodal Biomarkers Discovery in Kidney Disease using High Spatial and Spectral Resolution Mass Spectrometry Imaging;** Satoshi Miyamoto^{2,3}; Gregory Hamm¹; David Bonnel¹; Kumar Sharma^{2,3}; Jonathan Stauber¹; ¹*ImaBiotech, MS Imaging Dept., LOOS, France*; ²*Institute of Metabolomic Medicine, San Diego, CA*; ³*Center for Renal Translational Medicine, Division, San Diego, CA*

TOH am 09:30 **Tracking Metabolomic Dynamics during Corn Seed Germination using MALDI Mass Spectrometry Imaging;** Adam Feenstra^{1,2}; Andy Korte^{1,2}; Young-Jin Lee^{1,2}; ¹*Iowa State University, Ames, IA*; ²*Ames Laboratory, Ames, IA*

TOH am 09:50 **Spatial Metabolomics of Alzheimer's Disease Brains using LAESI-MS;** Greg Kilby²; Callee Walsh²; Pamela Cantrell²; Greg Boyce²; James Langridge¹; Giuseppe Astarita¹; ¹*Waters Corporation, Milford, MA*; ²*Protea Biosciences, Morgantown, WV*

TOH am 10:10 **Imaging Mass Spectrometry of 3D Cell Cultures: Novel Approach to Evaluate the Penetration of New Therapeutics and Apoptotic Imaging Probes;** Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*

10:30 AM – 2:30 PM, TUESDAY

TUESDAY POSTER SESSION

Poster/Exhibit Hall

Lunch concessions are open 11:00 am – 2:00 pm

TUESDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, TUESDAY AFTERNOON
SPACE SCIENCE, ASTROBIOLOGY, AND
ATMOSPHERIC CHEMISTRY

Jos Oomens (Radboud University), presiding
Exhibit Hall AB

TOA pm 2:30 **Detection of Organics in Geological Samples Containing Perchlorate with the MOMA Linear Ion Trap Mass Spectrometer;** Ricardo Arevalo Jr.¹; Xiang Li²; Veronica Pinnick²; Friso H.W. Van Amerom³; Ryan M. Danell⁴; Stephanie Getty¹; Lars Hovmand⁵; Paul Mahaffy¹; William Brinckerhoff¹; Fred Goesmann⁶; Harald Steining⁶; ¹*NASA GSFC, Greenbelt, MD*; ²*University of Maryland, Baltimore County, Greenbelt, MD*; ³*SRI International, Hyattsville, MD*; ⁴*Danell Consulting, Inc., Winterville, NC*; ⁵*Linear Labs LLC, Washington, DC*; ⁶*MPS, Lindau, Germany*

TOA pm 2:50 **Label-Free Quantitation and Dynamic SILAC to Investigate the Effects of Microgravity on Primary Cardiac Cells;** J. Will Thompson¹; Bryan J. Feger¹; Laura G. Dubois¹; Matthew W. Foster¹; Lisa Scott Carnell²; Dawn E. Bowles¹; M. Arthur Moseley¹; ¹*Duke University School of Medicine, Durham, NC*; ²*NASA Langley Research Center, Hampton, VA*

TOA pm 3:10 **Identification and Separation of Oxidized Organic Aerosol Precursors using a Novel Field-Deployable High Resolution Ion Mobility Time-of-Flight Mass Spectrometer (IMS-TOF);** Jordan Krechmer¹; Manjula Canagaratna²; Joel Kimmel^{2,3}; Heikki Junninen⁴; Richard Knochenmuss³; Mike Cubison³; Paola Massoli²; Harald Stark^{1,2}; John T. Jayne²; Jason Surratt⁶; Jose L. Jimenez¹; Douglas Worsnop^{2,4}; ¹*University of Colorado, Boulder, CO*; ²*Aerodyne Research Inc., Billerica, MA*; ³*Tofwerk, AG, Thun, Switzerland*; ⁴*University of Helsinki, Helsinki, Finland*; ⁵*University of North Carolina, Chapel Hill, NC*

TOA pm 3:30 **Proteome Expression Profiling of Hypergravity Exposure in Drosophila: Preparing for a NASA Space Mission;** Ravikumar Hosamani²; Chris Adams¹; Shilpa R. Bhardwaj²; Anna Okumu¹; Allis S. Chien¹; Sharmila Bhattacharya²; ¹*Stanford University Mass Spectrometry, Stanford, CA*; ²*NASA Ames, Sunnyvale, CA*

TOA pm 3:50 **Reactions of N-containing PAH Anions with N and O atom: A DFT Study of Processes of Interstellar Interest;** Zhechen Wang^{1,2}; Veronica M. Bierbaum^{1,2}; ¹*University of Colorado, Boulder, CO*; ²*University of Colorado, Boulder, CO*

TUESDAY AFTERNOON ORAL SESSIONS

TOA pm 4:10 **Prebiological Evolution of Macromolecules. Investigation of the Abiogenic Peptide Formation at the Different Conditions by High Resolution Mass Spectrometry;** Alexey Kononikhin^{1,2}; Olga Demina¹; Igor Popov^{1,2}; Natalia Starodubtseva^{1,2}; Alexey Boldyrev²; Andrey Khodonov¹; Sergey Varfolomeev¹; Eugene Nikolaev^{1,2}; ¹Emanuel Institute of Biochemical Physics, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia

2:30 – 4:30 PM, TUESDAY AFTERNOON NANO-SCALE AND MICROFLUIDIC SEPARATIONS AND MASS SPECTROMETRY

Bryan Fonslow (Scripps Research Institute), presiding
Room 307-308

TOB pm 2:30 **Next Generation Blood Sampling For Mass Spectral Analysis Of Proteins and Metabolites;** Fred Regnier¹; Tim Woenker²; JinHee Kim²; Jiri Adamec³; ¹Purdue University, West Lafayette, IN; ²Novilytic Laboratories, West Lafayette, Indiana; ³University of Nebraska, Lincoln, NE

TOB pm 2:50 **Peering into Biology from the Outside: Exometabolic Microfluidics-Based Platforms Integrated with Structural Mass Spectrometry for Systems, Synthetic, and Chemical Biology;** John A. Mclean; Stacy D. Sherrod; Cody R. Goodwin; Virginia Pensabene; John P. Wiksw; *Vanderbilt University, Nashville, TN*

TOB pm 3:10 **High Peak Capacity Ultranarrow PLOT LC Columns Coupled to Mass Spectrometry for Proteomic Analysis of Vanishingly Small Samples;** Barry L. Karger¹; Siyang Li¹; Xianzhe Wang¹; Shashi K. Murthy¹; David Fenyo²; Alexander R. Ivanov¹; ¹Barnett Institute, Northeastern University, Boston, MA; ²New York University, New York, NY

TOB pm 3:30 **High Resolution HILIC for Proteomic LC-MS;** Kanta Horie^{1,2}; Takeo Kamakura¹; Suguru Ichihara¹; Masaki Wakabayashi¹; Nobuo Tanaka³; Yasushi Ishihama¹; ¹Kyoto University, Kyoto, Japan; ²Eisai Co., Kawashima, Japan; ³GL Sciences, Iruma, Japan

TOB pm 3:50 **Capillary Zone Electrophoresis-Electrospray Ionization-Tandem Mass Spectrometry for Highly Sensitive Shotgun Proteomics;** Liangliang Sun; Guijie Zhu; Xiaojing Yan; Si Mou; Norman J. Dovichi; *University of Notre Dame, South Bend, IN*

TOB pm 4:10 **A Hybrid Microchip/Capillary Electrophoresis Mass Spectrometry Platform for Rapid and Ultrasensitive Bioanalysis;** Ryan T. Kelly¹; Chengcheng Wang²; Cheng S. Lee²; Richard D. Smith¹; Keqi Tang¹; ¹Pacific NW National Laboratory, Richland, WA; ²University of Maryland, College Park, MD

2:30 – 4:30 PM, TUESDAY AFTERNOON PROTEIN-PROTEIN AND PROTEIN-LIGAND INTERACTIONS

Renato Zenobi, (ETH Zurich), presiding
Room 309-310

TOC pm 2:30 **Sheathless Capillary Electrophoresis Coupled with Mass Spectrometry in Analysis of Native Proteins and Protein Complexes;** Alexander R. Ivanov¹; Rosa Viner³; Marcia R. Santos²; David Horn M. ³; David R. Bush¹; Arseniy M. Belov¹; Barry L. Karger¹; ¹Barnett Institute, Northeastern University, Boston, MA; ²Sciex Separations, Brea, CA; ³Thermo Fisher Scientific, San Jose, CA

TOC pm 2:50 **Nanodiscs and CaR-ESI-MS: A Novel Method for the Discovery of Protein-Glycosphingolipid Interactions;** Aneika Leneay; Xuxin Fan; Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*

TOC pm 3:10 **Using Ion Mobility-Mass Spectrometry to Study the Interactions between Human Histone Deacetylase 8 and Poly-r(C)-binding Protein 1;** Shuai Niu; Byung Chul Kim; Carol Fierke; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*

TOC pm 3:30 **The Attainment of Low-Charge State HK97 Bacteriophage Capsid at 13 MTh using STJ Cryodetection MALDI Time-of-Flight Mass Spectrometry;** Jonathan Feldman¹; Robert Duda²; Roger Hendrix²; Mark E. Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA; ²University of Pittsburgh, Pittsburgh, Pennsylvania

TOC pm 3:50 **Electron Transfer Dissociation of Native Protein Complexes on a Quadrupole/Ion Mobility/TOF Instrument;** Frederik Lermlyte^{1,2}; Albert Konijnenberg¹; Jonathan P. Williams³; Jeff Brown³; Dirk Valkenburg^{2,4}; Frank Sobott^{1,2}; ¹University of Antwerp, Antwerpen, Belgium; ²CFP-CeProMa, University of Antwerp, Antwerp, Belgium; ³Waters Corporation, Manchester, UK; ⁴VITO, Mol, Belgium

TOC pm 4:10 **Towards a Molecular “Microscope”: MS-Based Identification of Endogenous Protein-Protein Interactions and Proximities using Global Chemical Stabilization in the Cellular Milieu;** Roman Subbotin; Brian Chait; *The Rockefeller University, New York, NY*

2:30 – 4:30 PM, TUESDAY AFTERNOON FUNDAMENTALS OF PEPTIDE FRAGMENTATION Yu Xia (Purdue University), presiding Room 314-317

TOD pm 2:30 **IRMPD Spectroscopy of Ammonia Complexes of Peptide Fragments;** Oscar Hernandez²; Philippe Maitre²; Bela Paizs¹; ¹Bangor University, Bangor, UK; ²Université Paris Sud, Paris, France

TOD pm 2:50 **ETD Performance Comparison among Benzyl/ Methyl/ n-Butylguanidine-Tagged Peptides;** Chang Xue; Jan Urban; František Tureček; *University of Washington, Department of Chemistry, Seattle, WA*

TOD pm 3:10 **Radical Additions to Aromatic Residues in Peptides Facilitate Unexpected Side Chain and Backbone Losses;** Xing Zhang; Ryan R. Julian; *University of California, Riverside, Riverside, CA*

TOD pm 3:30 **Understanding the Electron Capture Dissociation of Phosphopeptides by Use of Ion Mobility Mass Spectrometry and Molecular Dynamics Simulations;** Helen J. Cooper¹; Andrew W. Jones¹; Andrew J. Creese¹; Doyong Kim²; David H. Russell²; ¹University of Birmingham, Birmingham, UK; ²Texas A&M University, College Station, Texas

TOD pm 3:50 **Enhanced Loss of Phosphate from Isobarically Tagged Phosphotyrosine Peptides: Impact on Site Localization Assignment, Immonium Ion Formation and MS/MS Interpretation;** Robert A. Everley¹; Edward L. Hutlin¹; Sean A. Beausoleil²; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA; ²Cell Signaling Technology, Danvers, MA

TOD pm 4:10 **Applying Arginylation for Proteomics;** H. Alexander Ehardt; Ruedi Aebersold; *ETH Zurich, Zurich, CH*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
TOP-DOWN PROTEIN ANALYSIS**
Jeff Agar (Northeastern University), presiding
Ballroom I, level 4

TOE pm 2:30 **Top Down Ultraviolet Photodissociation For Confirmation of Linkage Specificity of Polyubiquitin Chains;** Joe R. Cannon; Kirby Martinez-Fonts; Andreas Matouschek; Jennifer S. Brodbelt; *Univ. of Texas at Austin, Austin, TX*

TOE pm 2:50 **Intact Protein Characterization using Ultraviolet Photodissociation in a FT-ICR Mass Spectrometer;** Jared B. Shaw; Franklin E. Leach III; Tzu-Yung Lin; Si Wu; Errol W. Robinson; David W. Koppenaal; Ljiljana Paša-Tolić; *Pacific Northwest National Laboratory, Richland, WA*

TOE pm 3:10 **Probing the Structures of Protein Complexes up to 800 kDa by Native Top-Down Tandem Mass Spectrometry with FT-ICR;** Huilin Li¹; Jeremy Wolff²; Steve L. Van Orden²; Iain D G Campuzano³; Piriya Wongkongkathep¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; ¹*UCLA, Los Angeles, CA*; ²*Bruker Daltonics, Billerica, MA*; ³*Amgen Inc., Thousand Oaks, CA*

TOE pm 3:30 **Quantitation of Proteoform-Level Responses in Oncogene-Induced Senescence using Label-free Top Down Proteomics and Advanced Data Acquisition;** Kenneth Durbin; Ryan Fellers; Paul Thomas; Philip Compton; Neil L. Kelleher; *Northwestern University, Evanston, IL*

TOE pm 3:50 **Investigating Redox Regulation in the Apoptotic Pathway using High Resolution Mass Spectrometry;** Sophie Thurlow; David Clarke; Pat Langridge-Smith; C. Logan Mackay; Colin Campbell; *Edinburgh University, Edinburgh, UK*

TOE pm 4:10 **Quantitation of Histones H2A/H2B and Their Changes during Biological Events by Top-Down FT-ICR MS/MS Analysis;** Xibei Dang¹; Brian D. Spetman¹; Krystal D. Nolan²; Jennifer S. Isaacs²; Jonathan H. Dennis¹; Alan G. Marshall³; Nicolas L. Young³; ¹*Florida State University, Tallahassee, FL*; ²*Medical University of South Carolina, Charleston, SC*; ³*National High Magnetic Field Laboratory, Tallahassee, FL*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
DRUG TARGET DISCOVERY AND VALIDATION**

Jim Glick (Novartis BioMedical Research Institute), presiding
Ballroom II, level 4

TOF pm 2:30 **Dissecting the Binding Mode of Low Affinity Phage Display Ligands by Hydrogen/Deuterium Exchange Mass Spectrometry;** Ulrike Leurs¹; Rasmus Clausen¹; Brian Lohse¹; Jesper Kristensen¹; Kasper D. Rand²; ¹*University of Copenhagen, Copenhagen, Denmark*; ²*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*

TOF pm 2:50 **Impacting Translation of Biotherapeutics with Immunoaffinity LC-MS/MS Quantification of Protein Targets;** Joe Palandra; Hendrik Neubert; *Pfizer, Andover, MA*

TOF pm 3:10 **Central Dogma of Proteomics Provides Identification of Protein Targets, Action Mechanisms and Cellular Death Pathways of Small Molecule Anticancer Drugs;** Consuelo Marin Vicente^{1,2}; Mohammad Pirmoradian¹; Bo Zhang¹; Alexey Chernobrovkin¹; Neus Visa²; Roman Zubarev¹; ¹*Karolinska Institute, Stockholm, Sweden*; ²*Stockholm University, Stockholm, Sweden*

TOF pm 3:30 **Affinity Selection - High Resolution Mass Spectrometry Screening to Rapidly Assess Druggability in the NF-kappaB Pathway;** Christine L. Andrews; Victoria Kutilek; Matthew Richards; Elliott Nickbarg; Michael Ziebell; Ryan Boinay; Chad Chamberlin; Patrick Curran; Peter Saradjian; Berengere Sauvagnat; Xianshu Yang; Nadya Smotrov; Zangwei Xu; Peter Dandliker; Ilona Kariv; Bruce Beutel; *Merck, Boston, MA*

TOF pm 3:50 **Ion Mobility-Mass Spectrometry for Screening Amyloid Formation Inhibitors within Rationally-Designed Bifunctional Small Molecule Libraries;** Richard Kerr¹; Jeffrey S. Derrick¹; Michael W. Beck¹; Younwoo Nam²; Mi Hee Lim²; Brandon Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Ulsan National Institute of Science and Technology, Ulsan, South Korea*

TOF pm 4:10 **Successful High-Throughput Affinity-Selection Mass Spectrometry Assays of Mixtures of 200 Compounds by Time-of-Flight LCMS;** Mark Bean; Christopher Kwiatkowski; Sunny Hung; Stacy O'Neil Slawecky; Matt Kowalski; Geoffrey Quinque; Larry Szewczuk; Matt Zajac; *GlaxoSmithKline, Collegeville, PA*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
CLINICAL DIAGNOSTICS**
Tim Garrett (University of Florida), presiding
Ballroom III, level 4

TOG pm 2:30 **Development of on-Cartridge Enzyme Activity Assay for Cholinesterase in Human Whole Blood using Paper Spray Mass Spectrometry;** Yue Ren; Morgan McLuckey; Zheng Ouyang; *Purdue University, West Lafayette, IN*

TOG pm 2:50 **Targeted Metabolomics in Clinical Research Labs using LC-HRMS: Longitudinal Metabotype Determination for Individualized Biology in Healthy Volunteers;** Amélie Favre¹; Ronan Euzen¹; Marko Krstic¹; Olaf Scheibner²; Maciej Bromirski²; Pierre-Edouard Sottas³; Frédéric Schütz⁴; Bertrand Rochat¹; ¹*CHUV University Hospital, Lausanne, Switzerland*; ²*Thermo Fisher Scientific, Bremen, Germany*; ³*BioKaizen, Monthey, Switzerland*; ⁴*Swiss Institute of Bioinformatics, Lausanne, Switzerland*

TOG pm 3:10 **Validation of an Automated Immuno-MALDI Assay for the Clinical Measurement of Plasma Renin Activity;** Robert Popp¹; David Malmstrom¹; Alex Camenzind¹; Andrew Chambers¹; J Grace van der Gugten²; Daniel Holmes²; Christoph Borchers^{1,3}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; ²*St. Paul's Hospital, UBC, Vancouver, Canada*; ³*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*

TOG pm 3:30 **Translational Bionformatics Platform for Next Generation Histology by Imaging Mass Spectrometry**; [Kirill Veselkov](#)¹; Reza Mirnezami¹; Nicole Strittmatter¹; James Kinross¹; Abigail Speller¹; Tigran Abramov²; James McKenzie¹; Emrys Jones¹; Ara Darzi¹; Robert Goldin¹; Elaine Holmes¹; Jeremy Nicholson¹; Zoltan Takats¹; ¹*Imperial College, London, London*; ²*Sevastopol National Technical University, Sevastopol, Ukraine*

TOG pm 3:50 **An Empirically Driven Approach for the Identification of Optimal Peptides for Tandem Mass Spectrometry Experiments on Dried Blood Spots**; [James G. Bollinger](#); Clark M. Henderson; Andrew N. Hoofnagle; Michael J. MacCoss; *University of Washington, Seattle, WA*

TOG pm 4:10 **Universal Calibration: Populations Don't Lie, People Do**; [Matthew Crawford](#)¹; Christopher Shuford¹; Stacy Dee¹; Yvonne Wright¹; Martin Green¹; Patricia Holland¹; Mary Morr¹; Brian Rappold²; Russell Grant¹; ¹*LabCorp, Burlington, NC*; ²*Essential Testing, LLC, St. Louis, MO*

2:30 – 4:30 PM, TUESDAY AFTERNOON

IMAGING: FUNDAMENTALS, INSTRUMENTATION, AND METHOD DEVELOPMENT

Francisco Fernandez Lima (Florida International Univ.), presiding
Ballroom IV, level 4

TOH pm 2:30 **High-Resolution Tandem Mass Spectrometry Imaging**; [Bernhard Spengler](#); Dhaka Ram Bhandari; Andreas Römpf; *Analytical Chemistry, Giessen, Germany*

TOH pm 2:50 **New Developments in Nanospray Desorption Electrospray Ionization Mass Spectrometry: Compensation for Matrix Effects and Shotgun-like Quantification**; [Julia Laskin](#)^{1,2}; Ingela Lanekoff^{1,2}; ¹*Pacific NW National Laboratory, Richland, WA*; ²*Pacific NW National Laboratory, Richland, WA*

TOH pm 3:10 **Multimodal Imaging for Biological Applications: X-ray microCT and Mass Spectrometry Imaging**; [Anne Bruinen](#)¹; Shane Ellis¹; Enrico Schioppa²; Josef Uher³; Ron M.A. Heeren¹; Jan Visser²; ¹*FOM Institute AMOLF, Amsterdam, Netherlands*; ²*FOM institute Nikhef, Amsterdam, the Netherlands*; ³*Amsterdam Scientific Instruments, Amsterdam, the Netherlands*

TOH pm 3:30 **Coupling Atomic Force Microscopy with Biological Mass Spectrometry for High Spatial Resolution Imaging**; [Suman Ghorai](#); Chinthaka A. Seneviratne; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*

TOH pm 3:50 **Multi-modality 3-D Imaging of a Human Carotid Atherosclerotic Plaque: Correlating *in vivo* Ultrasound and Imaging Mass Spectrometry**; Heath Patterson¹; Martin Dufresne¹; Aurelien Thomas²; Robert James Doonan³; Stella Daskalopoulou³; [Pierre Chaurand](#)¹; ¹*University of Montreal, Montreal, Canada*; ²*University of Lausanne, Lausanne, Switzerland*; ³*McGill University Health Centre, Montreal, Canada*

TOH pm 4:10 **Soft-landing Ion Mobility Metal Deposition for MALDI-MS Imaging of Forensic and Biological Samples**; [Barbara Walton](#); Drew Sturtevant; Kent Chapman; Guido Verbeck; *University of North Texas, Denton, TX*

4:45 – 5:30 PM, TUESDAY AFTERNOON
AWARD LECTURE

Susan T. Weintraub (Univ. of Texas HSC, San Antonio), presiding
Exhibit Hall AB



Biemann Medal

Lingjun Li
University of Wisconsin-Madison

5:45 – 7:00 PM, TUESDAY AFTERNOON
WORKSHOPS

Level 3

Light refreshments, level 3

1. H/D Exchange, Covalent Labeling and Crosslinking (organized by H/D Exchange, Covalent Labeling & Cross Linking Interest Group); Room 307-308
2. LC-MS System Performance Tracking in LC-MS Tracking in LC-MS (organized by LC/MS & Related Topics Interest Group); Room 309-310
3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis (organized by Regulated Bioanalysis Interest Group); Room 314-317
4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment (organized by Analytical Lab Managers Interest Group); Room 336
5. FTMS: ICR and Orbitrap (organized by FTMS Interest Group); Room 337
6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry (organized by Environmental Applications Interest Group); Room 338
7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess (organized by Fundamentals Interest Group); Room 339-340
8. The NIH Review Process and Mock NIH Study Section; Room 341-342
9. Imaging Mass Spectrometry vs. Histology (organized by Imaging MS Interest Group); Room 343-344
10. Metabolomics: Emerging Technologies for Continued Innovation (organized by Metabolomics Interest Group); Room 345-346
11. 50 Years of the British Mass Spectrometry Society: Past, Present & Future; Room 347-348
12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud; Room 349-350

AFTER 8:00 PM, TUESDAY EVENING
CORPORATE HOSPITALITY SUITES
Hilton Hotel

**8:30 – 10:30 AM, WEDNESDAY MORNING
ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN SAMPLE
PREPARATION AND MS INTERFACE DESIGN**

**Mark Lowenthal (NIST), presiding
Exhibit Hall AB**

- WOA am 08:30 **Combining Metal Ion Complexation and Ultrahigh Resolution Mass Spectrometry for the Selective Analysis of Nitrogen Compounds in Asphaltenes;** Wolfgang Schrader; Sami Lababidi; *Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany*
- WOA am 08:50 **A Combined Experimental and Computational Study on the Reaction Pathways of Fast Pyrolysis of Cellobiose;** Mckay Easton; John Degenstein; Priya Murria; John J. Nash; Hilka I. Kenttamaa; *Purdue University, West Lafayette, IN*
- WOA am 09:10 **Detailed Characterization of Crude Oil and Its Fractions, Is Mass Spectrometry Sufficient?;** Michael T. Cheng; Matthew Hurt; *Chevron Research, Richmond, CA*
- WOA am 09:30 **Separation-Enhanced Characterization of Oxygenated Petroleum Compounds by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS);** Steven M. Rowland¹; Winston K. Robbins²; Yuri E. Corilo^{3,4}; Alan G. Marshall^{1,4}; Ryan P. Rodgers^{3,4}; ¹*FSU Department of Chemistry and Biochemistry, Tallahassee, FL*; ²*Consultant, Future Fuels Institute, FSU, Tallahassee, FL*; ³*Future Fuels Institute, Florida State University, Tallahassee, FL*; ⁴*Ion Cyclotron Resonance Program, NHMFL, FSU, Tallahassee, FL*
- WOA am 09:50 **Characterization and Quantification of Fermentation Inhibitors in Biomass Hydrolysates for Biofuel Production;** Arne Ulbrich; Alan J. Higbee; Samantha Austin; Daniel R. Noguera; John Ralph; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- WOA am 10:10 **Isomer Distribution Analysis for Improved Hydrocarbon Mixtures Characterization;** Aviv Amirav^{1,2}; Tal Alon^{1,2}; Alexander Fialkov¹; ¹*Tel-Aviv University, Tel-Aviv, Israel*; ²*Aviv Analytical Ltd, Tel Aviv, Israel*

**8:30 – 10:30 AM, WEDNESDAY MORNING
AMBIENT AND ATMOSPHERIC PRESSURE
IONIZATION: FUNDAMENTALS**

**Brian Clowers (Washington State University), presiding
Room 307-308**

- WOB am 08:30 **Evaluation of Nanopipette Emitters with Orifice Diameters Less Than 100 Nanometers for Use in Electrospray Ionization Mass Spectrometry;** Steven Ray¹; Elizabeth Yuill¹; Alicia Friedman¹; Anumita Saha¹; Chris Enke²; Gary Hieftje¹; Lane Baker¹; ¹*Indiana University, Bloomington, IN*; ²*University of New Mexico, Albuquerque, NM*
- WOB am 08:50 **Fundamental Spray Characteristics and Complex Formation using SAWN and Other Spray Techniques;** Bob Hommersom¹; Shane R. Ellis¹; Tiffany Porta¹; Marc C. Duursma¹; Yue Huang²; Scott R. Heron²; David R. Goodlett²; Ron M.A. Heeren¹; ¹*FOM Institute AMOLF, Amsterdam, Nederland*; ²*University of Maryland, Baltimore, MD*

WOB am 09:10 **Supercharging Techniques for Protein Desalting and Structural Characterization from Native Aqueous Solutions;** Catherine A. Cassou; Evan R. Williams; *University of California, Berkeley, Berkeley, CA*

WOB am 09:30 **Evolution of Ions from Charged Droplets Studied by Pulsed Nanospray Coupled to Ion Mobility-Mass Spectrometry;** Carina Minardi; Kaveh Jorabchi; *Georgetown Univ., Washington, DC*

WOB am 09:50 **Surprising New Ionization Methods for Mass Spectrometry, Mechanistic Insights and Potential Practical Utility;** Sarah Trimpin; Corinne Lutomski; Tarick El-Baba; Beixi Wang; Lorelie Imperial; Daniel Woodall; Ruby Kumar; Bryan Harless; Casey Foley; Chih-Wei Liu; Ellen Inutan; *Wayne State University, Detroit, MI*

WOB am 10:10 **Optical Spectroscopic Comparisons of Helium Plasma Ambient Desorption/Ionization Sources for Mass Spectrometry;** Paul Farnsworth¹; Wade Ellis¹; Charlotte Reininger¹; Joel Keelor²; Adam Kaylor²; ¹*Brigham Young University, Provo, UT*; ²*Georgia Institute of Technology, Atlanta, GA*

**8:30 – 10:30 AM, WEDNESDAY MORNING
THE TRIPLE QUADRUPOLE 35 YEARS ON EVOLUTION AND
APPLICATIONS TO CELEBRATE CHRIS ENKE'S 80TH BIRTHDAY
R. Graham Cooks (Purdue University), presiding
Room 309-310**

- WOC am 08:30 **The Triple Quadrupole: An Historical Perspective;** Richard A. Yost; *University of Florida, Gainesville, FL*
- WOC am 08:50 **The Secret Identity of Phase-Space 'Ellipses' – Are They Misnamed?;** David P.A. Kilgour¹; David R. Goodlett¹; John F.J. Todd²; ¹*School of Pharmacy, University of Maryland, Baltimore, MD*; ²*School of Physical Sciences, University of Kent, Canterbury, UK*
- WOC am 09:10 **Mass Selective Axial Ejection in a Low Pressure Linear Ion Trap in the presence of Nonlinear RF Fields;** Mircea Guna; *AB Sciex, Concord, Canada*
- WOC am 09:30 **Moore's Law and the Consequence of Technological Change;** Alan Schoen; *Thermo Fisher Scientific, San Jose, CA*

WOC am 09:50 **Performance Investigation and Mass Resolution Enhancement of an Electrospray Ionization Quadrupole Mass Spectrometer with a Position Sensitive Detector;** Sarfaraz Syed; Gert Eijkel; Shane Ellis; Donald Smith; Ron Heeren; *FOM Institute AMOLF, Amsterdam, The Netherlands*

WOC am 10:10 **Room for Improvement;** Christie G. Enke; *University of New Mexico, Placitas, NM*

**8:30 – 10:30 AM, WEDNESDAY MORNING
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY/CELLULAR
PATHWAY ANALYSIS**

**Michael Fitzgerald (Duke University), presiding
Room 314-317**

- WOD am 08:30 **Metastatic Potential of Osteosarcoma Cells Mapped through Kinase Networks;** Ievgen Motorykin; Milan Milovancev; Shay Bracha; Marcus Weinman; Claudia Maier; *Oregon State University, Corvallis, OR*

WOD am 08:50 **Measuring Reduced-Representation Phosphorylation Profiles with a High-Throughput MS Assay Produces a “Connectivity Map” of Signaling Responses to Drug Perturbations;** Jennifer G. Abelin; Jinal Patel; Lola Fagbami; Xiaodong Lu; Steven A. Carr; Jacob D. Jaffe; *Broad Institute of MIT and Harvard, Cambridge, MA*

WOD am 09:10 **Integration of Ribosome Profiling with Label-Free Quantitative Proteomics;** Andy Kong; Chih-Chiang Tsou; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*

WOD am 09:30 **Transformation of Mouse Embryonic Stem Cells to extra-Embryonic Endoderm (XEN) cells: A Proteomic Investigation of Early Cell Fate Decision Making;** Claire Mulvey^{1,2}; Christian Schröter²; Laurent Gatto¹; Mike Deery¹; Kathy Niakan³; Alfonso Martinez-Arias²; Kathryn S. Lilley¹; ¹*Dept. of Biochemistry, University of Cambridge, Cambridge, U.K.*; ²*Dept. of Genetics, University of Cambridge, Cambridge, U.K.*; ³*MRC NIMR, Mill Hill, London, U.K.*

WOD am 09:50 **Cross-Omics: Global Phosphoproteomics and Metabolomics Reveals a Connection between Kinase Inhibition and RNA Processing in BCR-ABL H929 Myeloma Cells;** Susanne Breikopf^{1,2}; Min Yuan¹; Katja Helenius^{1,2}; Costas Lyssiotis³; John M Asara¹; ¹*Beth Israel Deaconess Medical Center, Boston, MA*; ²*Harvard Medical School, Boston, MA*; ³*Weill Cornell Medical College, New York, NY*

WOD am 10:10 **NeuCode Mouse: Multiplexed Proteomic Analysis Reveals Tissue Specific Effects of Deubiquitinase Deletion;** Christopher M. Rose¹; Joshua M. Baughman²; Timothy W. Rhoads¹; Clay E. Williams¹; Anna E. Merrill¹; Donald S. Stapleton¹; Mark P. Keller¹; Alexander S. Hebert¹; Michael W. Westphall¹; Alan D. Attie¹; Donald S. Kirkpatrick²; Anwesha Dey²; Joshua J. Coon¹; ¹*University of Wisconsin, Madison, WI*; ²*Genentech, South San Francisco, CA*

**8:30 – 10:30 AM, WEDNESDAY MORNING
PEPTIDOMICS**

**Amanda Hummon (University of Notre Dame), presiding
Ballroom I, level 4**

WOF am 08:30 **Distinct Peptidome Signatures of Triple Negative Breast Cancer Revealed by Large-Scale Comparative Peptidomic Analysis;** Chaochao Wu; Zhe Xu; Fang Xie; Athena Schepmoes; Thomas Fillmore; Rosalie Chu; Gordon Slysz; Matthew Monroe; Ronald Moore; Yufeng Shen; Nikola Tolic; Samuel Payne; David Camp; Tao Liu; Richard Smith; *Pacific Northwest National Laboratory, Richland, WA*

WOF am 08:50 **Peptidomics of Human Milk during Lactation and Mastitis;** Stephanie Contreras; Andres Guerrero; Dave Dallas; Lauren Wu; Jennifer Smilowitz; Daniela Barile; Bruce German; Carlito Lebrilla; *University of California, Davis, Davis, CA*

WOF am 09:10 **Mass Spectral Investigation of Circadian Rhythm-Related Neuropeptide Secretion in Crustacean via *in vivo* Microdialysis;** Zhidan Liang¹; Claire Schmerberg²; Lingjun Li¹; ¹*UW-Madison, Madison, Wisconsin*; ²*Duke University, Durham, NC*

WOF am 09:30 **Investigating Mechanism of Preeclampsia by Probing Low Molecular Weight (LMW) Placental Proteome using Capillary Liquid Chromatography-Time-Of-Flight Mass Spectrometer (cLC/Q-ToF);** Komal Kedia; Steven Graves; Craig Thulin; Bruce Jackson; *BYU, Provo, Utah*

WOF am 09:50 **Analytical Strategy for the High-Throughput Sequencing of Venom Peptides (1-10kDa) Combining Cutting-Edge Technologies of Proteomics, Transcriptomics and Bioinformatics;** Loïc Quinton¹; Michel Degueudre¹; Julien Echterbille¹; Marion Verdenaud²; Madeleine Boulanger¹; Charlotte Gouin³; Jordi Durban⁴; Raquel Rodriguez⁴; Rebeca Minambres⁴; Frederic Ducancel²; Nicolas Gilles³; Edwin De Pauw¹; ¹*Laboratory of mass spectrometry, ULg, Liège, Belgique*; ²*iBiTEc S/SPI Antibody Eng. for Health, Gif-sur-Yvette, France*; ³*iBiTEcS, SIMOPRO, Gif-sur-Yvette, France*; ⁴*Sistemas Genomicos Ltd, Valencia, Spain*

WOF am 10:10 **Expanding the Detectable HLA Peptide Repertoire using Electron-Transfer / Higher-Energy Collision Dissociation (ETHcD);** Geert P.M. Mommen¹; Christian K. Frese²; Hugo D. Meiring¹; Jacqueline van Gaans-van den Brink³; Ad P.J.M. de Jong¹; Cecile A.C.M. van Els³; Albert J.R. Heck²; ¹*Intravacc, Bilthoven, Netherlands*; ²*Utrecht University, Utrecht, Netherlands*; ³*RIVM, Bilthoven, Netherlands*

**8:30 – 10:30 AM, WEDNESDAY MORNING
PHARMACOPROTEOMICS AND TOXICOPROTEOMICS FOR
DRUG DEVELOPMENT**

**Alexander Ivanov (Northeastern University), presiding
Ballroom II, level 4**

WOF am 08:30 **High Resolution LC/MS-based Background Subtraction for Toxicoproteomic Profiling: Application to Differentiate Microsomal Protein Bindings of Acetaminophen versus Those of 3-hydroxyacetanilide;** Haiying Zhang; Jinping Gan; Yue-Zhong Shu; W. Griffith Humphreys; *Bristol-Myers Squibb R&D, Princeton, NJ*

WOF am 08:50 **Absolute Quantitation of NAPQI-modified Serum Albumin from Rat Plasma Samples by LC-MS/MS: Monitoring Acetaminophen Toxicity;** André Leblanc; Tze Chieh Shiao; René Roy; Lekha Sleno; *UQAM, Montreal, Canada*

WOF am 09:10 **Direct Monitoring of Protein-Protein Inhibition Using Nano Electrospray Ionization Mass Spectrometry;** Dragana Cubrilovic¹; Konstantin Barylyuk¹; Daniela Hofmann¹; Martin Gräber²; Thorsten Berg²; Gerhard Wider¹; Renato Zenobi¹; ¹*ETH Zurich, Zurich, Switzerland*; ²*Universität Leipzig, Leipzig, Germany*

WOF am 09:30 **Tandem Mass-Spectrometry on Native Non-Reduced and Reduced Antibody-Drugs Conjugates using an Orbitrap Mass Spectrometer Equipped with a High-Mass Quadrupole;** Andrey Dyachenko^{1,2}; Sara Rosati^{1,2}; Mike Belov³; Eugen Damoc³; Eduard Denisov³; Alexander Makarov^{1,3}; Albert Heck^{1,2}; ¹*University of Utrecht, Utrecht, Netherlands*; ²*Netherlands Proteomics Center, Utrecht, Netherlands*; ³*ThermoFisher Scientific, Bremen, Germany*

WOF am 09:50 **More from Less: Straightforward Turn-Key Workflow Enables Combined Pharmacokinetic and Integrated "Omic" Studies from Limited Tissue**; Jon Reed^{1,2}; Gogce Crynen^{1,2}; Laila Abdullah^{1,2}; Ariel Hart¹; Prashanthi Vallabhaneni¹; Rosa Joy¹; Daniel Paris^{1,2}; Fiona Crawford^{1,2}; ¹Roskamp Institute, Sarasota, Florida; ²SRQ Bio, Sarasota, Florida

WOF am 10:10 **Full Structure Elucidation of Elapid Snake Venom Proteins Targeting the Acetylcholine Receptor using the latest Quadrupole-Orbitrap Mass Spectrometer**; Martijn Pinkse¹; Jeroen Kool²; Laurens van Herpen¹; Tabiwang Arrey³; Markus Kellmann³; Peter D. Verhaert¹; ¹Delft University of Technology, Delft, Netherlands; ²VU University Amsterdam, Amsterdam, Netherlands; ³Thermo Fisher Scientific, Bremen, Germany

**8:30 – 10:30 AM, WEDNESDAY MORNING
PTMS: COMPREHENSIVE ANALYSIS**

**Saiful Chowdhury (University of Texas, Arlington), presiding
Ballroom III, level 4**

WOG am 08:30 **Middle-Down Proteomics Reveals Interdependency of Histone Marks and Assists Their Functional Characterization**; Simone Sidoli¹; Veit Schwämmle¹; Xudong Wu²; Chung-Fan Lee²; Kristian Helin²; Ole Nørregaard Jensen¹; ¹University of Southern Denmark, Odense, Denmark; ²Centre for Epigenetics, BRIC, Copenhagen, Denmark

WOG am 08:50 **Global Ubiquitylome Profiling for the Identification of Oncogenic Effector Substrates and Drug Targets in Cancer**; Namrata Udeshi¹; Jean-Philippe Theurillat^{1,2}; Jan Krönke³; Tanya Svinkina¹; Monica Schenone¹; Benjamin Ebert^{1,3}; Levi Garraway^{1,2}; Steven A. Carr¹; ¹The Broad Institute of MIT and Harvard, Cambridge, MA; ²Dana-Farber Cancer Institute, Boston, MA; ³Brigham and Women's Hospital, Boston, MA

WOG am 09:10 **An Ultra-tolerant Database Search Identifies Hundreds of Thousands of Modified Peptides**; Joel Chick; David Nusinow; Bo Zhai; Steven P. Gygi; Harvard medical school, Boston, MA

WOG am 09:30 **Comprehensive Monitoring of Dynamic Phosphorylation on Intact Proteins by Native MS on an Extended Mass Range Orbitrap**; Michiel Van De Waterbeemd¹; Philip Lössl¹; Violette Gautier¹; Masami Yamashita²; Elena Conti²; Albert J.R. Heck¹; ¹Utrecht University, Utrecht, The Netherlands; ²Max Planck Institute of Biochemistry, Martinsried, Germany

WOG am 09:50 **Lysine 2-Hydroxyisobutyrylation is a New and Widely Distributed Histone Modification with Important Biological Functions**; Lunzhi Dai¹; Chao Peng¹; Emilie Montellier²; Zhike Lu¹; Yue Chen¹; Haruhiko Ishii⁴; Alexandra Debernardi²; Thierry Buchou²; Sophie Rousseaux²; Fulai Jin⁴; Benjamin R. Sabari³; Zhiyou Deng¹; He Huang¹; C. David Allis³; Bing Ren⁴; Saadi Khochbin²; Yingming Zhao¹; ¹University of Chicago, Chicago, Illinois; ²Université Joseph Fourier, La Tronche Cedex, France; ³The Rockefeller University, New York, NY; ⁴University of California, San Diego, La Jolla, CA

WOG am 10:10 **Novel Acyl-Lysine Modifications in a Bacterial Proteome Elucidate Substrate Metabolism**; Hong Hanh Nguyen¹; Yanan Yang¹; Robert Gunsalus¹; Michael McInerney²; Joseph Loo¹; Rachel Ogorzalek Loo¹; ¹UCLA, Los Angeles, CA; ²The University of Oklahoma, Norman, OK

**8:30 – 10:30 AM, WEDNESDAY MORNING
LIPIDS AND PROFILING**

**Kim Ekroos (Zora Biosciences), presiding
Ballroom IV, level 4**

WOH am 08:30 **Functional Lipidomics - From Structural Characterization to Regulation of Lipid Metabolic Networks**; Christer Ejsing; *Department Of Biochemistry And Molecular Biology, Odense, Denmark*

WOH am 08:50 **Stable Isotope Labeling in Cell Culture of Short-, Medium- and Long-Chain acyl-Coenzyme A Thioesters for SID-LC-MS/MS Analysis**; Nathaniel W. Snyder; Sankha S. Basu; Zinan Zhou; Andrew J. Worth; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*

WOH am 09:10 **Biosynthetic Pathway of 12-hydroxyheptadecatrienoic Acid Revealed by LC-MS/MS System**; Toshiaki Okuno¹; Takehiko Matsunobu²; Takehiko Yokomizo¹; ¹Department of Biochemistry, Juntendo University, Tokyo, Japan; ²Medical Biochemistry, Kyushu University, Fukuoka, Japan

WOH am 09:30 **Method Development for Comprehensive Analysis of Lysophospholipid Molecular Species by Shotgun Lipidomics**; Chunyan Wang; Miao Wang; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*

WOH am 09:50 **Single-Cell Nanomanipulation to Identify Lipid Heterogeneity in Mammalian Cells at the Cancer Forefront**; Jason Hamilton; Mandy Phelps; Guido Verbeck; *University of North Texas, Denton, TX*

WOH am 10:10 **Glucosylceramide and Glucosylsphingosine Quantitation by Liquid Chromatography-Tandem Mass Spectrometry to Enable Studies of Neuronopathic Gaucher Disease**; Rick Hamler; Nastry Brignol; Sean Morrison; Hui Chang; Leo Dungan; Robert Boyd; Sean Clark; Richie Khanna; John Flanagan; Kenneth Valenzano; Elfrida Benjamin; *Amicus Therapeutics, Cranbury, New Jersey*

**10:30 AM – 2:30 PM, WEDNESDAY
WEDNESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm**

WEDNESDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, WEDNESDAY AFTERNOON ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN MS DESIGN AND INFORMATICS

**Michael Freitas (Ohio State University), presiding
Exhibit Hall AB**

WOA pm 2:30 **Elucidating Structures of Compounds in Complex Mixture by a Combination of Ion Mobility and Ultrahigh-Resolution MS and Collisional Cross-Section Calculation;** Sunghwan Kim¹; Ahmed Arif¹; Eleanor Riches²; Kevin Giles²; Yunju Cho¹; Hugh I Kim³; Jong Wha Lee³; Cheol Ho Choi¹; ¹Chemistry Department, Kyungpook National University, Daegu, South Korea; ²Waters Corporation, Manchester, N/A; ³Pohang University of Science and Technology, Pohang, Republic of Korea

WOA pm 2:50 **Ion Mobility Petroleomics: Towards Isomeric Compositional Space Elucidation via New Software and Methods;** Eleanor Riches¹; Priscilla Lalli²; Ryan P. Rodgers^{2,3}; Yuri Corilo^{2,3}; ¹Waters Corporation, Wilmslow, UK; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Future Fuels Institute, Tallahassee, FL

WOA pm 3:10 **Analysis of Crude Oil Samples on the Multi Reflecting High Resolution TOF at resolution over 160,000;** George Tikhonov¹; Viatcheslav Artaev¹; Boris Kozlov²; Kevin Siek¹; Anatoly Verenchikov²; ¹LECO Corporation, Saint Joseph, MI; ²MS Consulting, Bar, Montenegro

WOA pm 3:30 **Direct Analysis of Crude Oil using Orbitrap Mass Spectrometry with Resolving Powers above 1,000,000;** Eduardo M. Schmidt¹; Marcos A. Pudenzi¹; Jandyson M. Santos¹; Eugen Damoc²; Eduard Denisov²; Alexander Makarov²; Marcos N. Eberlin¹; ¹ThermoFisher Mass Spectrometry Laboratory, Campinas, Brazil; ²Thermo Fisher Scientific, Bremen, Germany

WOA pm 3:50 **Spectroscopic and FT-ICR Mass Spectral Analysis of Asphaltene Subfractionation by N-Methyl-2-pyrrolidone;** Mmili M. Mapolelo¹; Simon I. Andersen¹; Amy M. McKenna²; Jacqueline M. Jarvis²; Ryan P. Rodgers²; Alan G. Marshall²; ¹Schlumberger, Edmonton, Canada; ²Natl High Magnetic Field Laboratory, Tallahassee, FL

WOA pm 4:10 **Use of 2D GC-MS and ESI-FTICR-MS to Characterize Quality Crude Oil Produced from Aliphatic Coal via Hydrous Pyrolysis;** Blaine Hartman; Patrick Hatcher; Old Dominion University, Norfolk, VA

Maréchal²; Denis Falconet²; Akos Vertes¹; ¹George Washington University, Washington, District Of Columbia; ²CEA-CNRS-INRA-Univ. Grenoble Alpes, Grenoble, France

WOB pm 3:10 **Single-probe Sampling and Ionization Technique for Single Cell Mass Spectrometry Analysis: Development and Applications;** Ning Pan; Anthony Burgett; Naga Rama Kothapalli; Zhibo Yang; University of Oklahoma, Norman, OK

WOB pm 3:30 **High Repetition-Rate, Fiber-Based Laser Vaporization, Electrospray Ionization Mass Spectrometry (Fiber-LEMS);** Paul Flanagan¹; Fengjian Shi¹; Jieutonne Archer¹; Andrew Mills²; Martin Fermann²; Robert Levis¹; ¹Temple University, Philadelphia, PA; ²IMRA America, Inc., Ann Arbor, MI

WOB pm 3:50 **Direct Quantification of Chemical Warfare Agent Related Compounds using Active Capillary Inlet and SESI Mass Spectrometry;** Jan-Christoph Wolf¹; Pablo Martinez-Lozano Sinues¹; Martin Schaefer²; Renato Zenobi¹; ¹ETH Zurich, Zurich, CH; ²SPIEZ Laboratory, Spiez, CH

WOB pm 4:10 **jigSAWN: A Self-optimizing SAWN Control Interface;** Erik Nilsson²; Michael Wilson¹; Yue Huang¹; Scott Heron¹; David Kilgour¹; David Goodlett¹; ¹University of Maryland, Baltimore, Baltimore, MD; ²Deurion LLC, Seattle, WA

2:30 – 4:30 PM, WEDNESDAY AFTERNOON ECOLOGICAL AND HUMAN HEALTH ENVIRONMENTAL CHEMISTRY AND TOXICOLOGY

**J. Will Thompson (Duke University), presiding
Room 309-310**

WOC pm 2:30 **Comprehensive Characterization of Mixed-Halogen Dioxins and Furans Generated in Fire Debris Using GCxGC-TOFMS and APGC-TQS;** Kari Organtini¹; Anne Myers²; Karl Jobst³; Eric Reiner³; Jack Cochran⁴; Adam Ladak⁵; Douglas Stevens⁵; Frank Dorman¹; ¹Penn State University, University Park, PA; ²University of Toronto, Toronto, Canada; ³Ontario Ministry of the Environment, Toronto, ON; ⁴Restek Corporation, Bellefonte, PA; ⁵Waters Corporation, Beverly, MA

WOC pm 2:50 **Characterization of Paralytic Shellfish Poisons by HILIC-IM-MS coupling;** Salomé Poyer¹; Corinne Loutelier-Bourhis¹; Florence Mondeguer²; Julien Enche³; Gael Coadou¹; Anne Bossée³; Philipp Hess²; Carlos Afonso¹; ¹University of Rouen, Mont Saint Aignan, France; ²IFREMER, Nantes, France; ³DGA Maitrise NRBC, Vert Le Petit, France

WOC pm 3:10 **Fast Identification and Quantification of Major Protein Carbonyls α -amino adipic and γ -glutamic semialdehydes---A New Pronase Hydrolysis Methodology;** Lin Huang¹; Jacob Raber²; Claudia Maier¹; ¹Oregon State University, Corvallis, OR; ²Oregon Health & Science University, Portland, OR

WOC pm 3:30 **Supercritical Fluid Chromatography Coupled to Orbitrap Mass Spectrometry for Analysis of Oil Sands Process-Affected Water;** Alberto Pereira; Jonathan Martin; University of Alberta, Edmonton, Canada

2:30 – 4:30 PM, WEDNESDAY AFTERNOON

AMBIENT IONIZATION: INSTRUMENTATION AND APPLICATIONS

**Demian Ifa (York University), presiding
Room 307-308**

WOB pm 2:30 **Data-Independent Ion Correlations by Dynamic Sample Introduction Ambient MS;** Ezequiel M. Morzan¹; Rachel V. Bennett²; Facundo M. Fernandez²; ¹Universidad de Buenos Aires, Buenos Aires, Argentina; ²Georgia Institute of Technology, Atlanta, GA

WOB pm 2:50 **Metabolic Response to Altered Light Conditions in Genetically Modified Chlamydomonas by LAESI Mass Spectrometry with Ion Mobility Separation;** Sylvia Stopka¹; Bindesh Shrestha¹; Éric

WOC pm 3:50 **A Highly Sensitive, Fully Automated, High Throughput Method to Analyze Nicotine Metabolites in Human Serum using HPLC-APCI-Tandem Mass Spectrometry;** [Kristin Dortch](#); Kevin Caron; Hunter Ronald; Luo Zuzheng; Alexander Ricky; Akins Ricky; McGahee Ernest; Connie Sosnoff; Lanqing Wang; *Centers for Disease Control and Prevention, Atlanta, GA*

WOC pm 4:10 **Identification and Quantification of Fourteen N-Nitrosamines in Canadian Drinking Water Systems using SPE-HPLC-MS/MS Methods;** [Yichao Qian](#); Minghuo Wu; Jessica Boyd; Steve Hruddy; Xing-Fang Li; *University of Alberta, Edmonton, Canada*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
FUNDAMENTALS: NEW ION ACTIVATION METHODS
Hao Chen (Ohio University), presiding
Room 314-317**

WOD pm 2:30 **Improvement of the Low Mass Cutoff Effect using Digital Ion Trap Technology;** [Fuxing Xu](#); [Chuanfan Ding](#); *Fudan University, Shanghai, China*

WOD pm 2:50 **“Flow-Through” Electron Capture Dissociation in a Novel Branched Radio-Frequency Ion Trap for High Throughput Mass Spectrometry;** [Takashi Baba](#); J. Larry Campbell; Yves Le Blanc; Jim. W. Hager; Bruce A. Thomson; *AB Sciex, Concord, Canada*

WOD pm 3:10 **Effects of Sodium Cationization on Electron Detachment Dissociation Fragments of Heparin Oligosaccharides;** [Isaac Agvekum](#)²; Muchena J. Kailemia²; Lingyun Li³; Robert J. Linhardt³; Jon Amster¹; ¹*University of Georgia, Athens, GA*; ²*University of Georgia, Chemistry Department, Athens, GA*; ³*Rensselaer Polytechnic University, Troy, NY*

WOD pm 3:30 **UV Photogeneration of Peptidic Carbenes and UV Photodissociation of ETD Fragmentation Products;** [Christopher Shaffer](#); Ales Marek; Robert Pepin; Frantisek Turecek; *University of Washington, Seattle, Washington*

WOD pm 3:50 **Effect of Conformational Flexibility on Gas-Phase Unfolding of Noncovalent Protein Homodimers Probed by CID and SID;** [Yang Song](#); Yun Zhang; Royston Quintyn; Mowei Zhou; Vicki Wysocki; *The Ohio State University, Columbus, OH*

WOD pm 4:10 **Gas-Phase Structural Effects in Negative Ion Electron Capture Dissociation (niECD);** [Ning Wang](#); Kristina Hakansson; *University of Michigan, Ann Arbor, MI*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
PLANT“OMICS”
Ron Cerny (University of Nebraska), presiding
Ballroom I, level 4**

WOC pm 2:30 **Living Without Our Daily Bread – Towards Solutions for Sufferers of Gluten Intolerance;** [Michelle Colgrave](#)^{1,2}; Keren Byrne^{1,2}; Hareshwar Goswami^{1,2}; Greg Tanner^{2,3}; Crispin Howitt^{2,3}; ¹*CSIRO Animal, Food & Health Science, St Lucia, Australia*; ²*CSIRO Food Futures Flagship, Canberra, Australia*; ³*CSIRO Plant Industry, Black Mountain, Australia*

WOC pm 2:50 **Targeted and Nontargeted Apple Metabolomics using 96-blade LC-MS;** [Sanja Risticvic](#); Fatemeh Mousavi; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*

WOC pm 3:10 **Structural Identification of N-glycoproteins and Stress Signaling in Arabidopsis Thaliana;** Jun Ma; Qianqian Li; Guochen Qin; [Yi-Min She](#); *Shanghai Center for Plant Stress Biology, Shanghai, P. R. China*

WOC pm 3:30 **Nuclear Proteins Controlling Soybean Rust Resistance;** Bret Cooper; *USDA-ARS, Beltsville, MD*

WOC pm 3:50 **A Quantitative Systems Approach to Understand Differences in Geminivirus-induced Senescence in Arabidopsis thaliana;** [Laura Edwards](#); Inna Kulikova; Sophia Yang; Mariana Franco-Ruiz; Caroline Bryan; Elise Braswell; Lisa Rightmyer; Kevin Blackburn; Michael B. Goshe; Jose Trinidad Ascencio-Ibanez; *North Carolina State University, Raleigh, NC*

WOC pm 4:10 **Alteration of the Root Microbiome using Plant Mutants Affecting Root Carbon Allocation;** [Ljiljana Pasa-Tolic](#)¹; Charles Ansong¹; Joshua Aldrich¹; Heather Brewer¹; Alice Dohnalkova¹; Richard Ferrieri²; Susannah Green Tringe³; Michael Sadowsky⁴; Chanlan Chun⁴; Lihui Song⁵; Yaya Cui⁵; Vania Pankiewicz^{5,6}; Fernanda do Amaral^{5,7}; Karina Freire d’Eça Nogueira Santos^{5,6}; Emanuel de Souza⁵; Fabio Pedrosa⁵; Gary Stacey⁵; ¹*Pacific NW Nat’l Lab, Richland, WA*; ²*Brookhaven National Laboratory, Upton, NY*; ³*DOE Joint Genome Institute, Walnut Creek, CA*; ⁴*BioTechnology Institute, University of Minnesota, St. Paul, MN*; ⁵*University of Missouri, Columbia, MO*; ⁶*Federal University of Parana, Curitiba, Brazil*; ⁷*Federal University of Santa Catarina, Florianopolis, Brazil*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
PROTEOMICS: INFECTIOUS DISEASES
Rena Robinson (University of Pittsburgh), presiding
Ballroom II, level 4**

WOF pm 2:30 **Identification of HLA-DR-Presented Peptides in Synovial Tissue and Fluid, and PBMCs from Patients with Rheumatoid Arthritis or Antibiotic-Refractory Lyme Arthritis;** [Qi Wang](#)¹; Elise E. Drouin²; Chunxiang Yao¹; Jiyang Zhang^{1,3}; Yu Huang¹; Allen C. Steere²; Catherine E. Costello¹; ¹*Boston University School of Medicine, Boston, MA*; ²*Massachusetts General Hospital, Boston, MA*; ³*National University of Defense Technology, Changsha, Hunan Province, China*

WOF pm 2:50 **Viral-induced Changes in the Liver Proteome;** Dijana Vitko; Anannya Bhattacharya; Katrin Hoermann; Katja Parapatics; André C. Mueller; Jacques Colinge; Andreas Bergthaler; [Keiryn L. Bennett](#); *CeMM Research Center for Molecular Medicine, Vienna, Austria*

WOF pm 3:10 **Revealing Essential Metabolic Enzymes for Mycobacterium Tuberculosis Survival using a Targeted Quantitation Strategy on a Q Exactive Mass Spectrometer;** [John D. Leszyk](#); Subhalaxmi Nambi; Scott A. Shaffer; Christopher Sasseti; *University of Massachusetts Medical School, Worcester, MA*

WOF pm 3:30 **Proteomic Identification of Interspecies Host-Pathogen Interactions by Protein Crosslinking: *Acinetobacter baumannii* Infection of Human Lung Epithelia;** Devin Schweppe; Juan Chavez; James Bruce; *University of Washington, Seattle, WA*

WOF pm 3:50 **Human Immune Defense versus Viral Immune Evasion: Emerging Roles for Phosphorylation and Acetylation in Virus-Host Dynamics;** Tuo Li; Benjamin Diner; Jin Chen; Ileana M. Cristea; *Princeton University, Princeton, NJ*

WOF pm 4:10 **Glycoproteomic Analysis of Plasmas from HIV Infected Individuals of Post-Seroconversion, with Developed AIDS, HAART and Elite Suppression;** Weiming Yang¹; Oliver Laeyendecker^{1,3}; Sarah Wendel²; Shisheng Sun¹; Jian-Ying Zhou¹; Minghui Ao¹; Joel Blankson²; Richard Moore²; George Seage III⁴; Connie Celum⁵; Deborah Donnell⁷; Susan Buchbinder⁶; Matthew Cousins¹; Hui Zhang¹; Jay Brooks Jackson¹; ¹*Department of Pathology, Johns Hopkins University, Baltimore, MD;* ²*Department of Medicine, Johns Hopkins University, Baltimore, MD;* ³*NIH, National Institutes of Health, Bethesda;* ⁴*Department of Epidemiology, Harvard SPH, Boston, MA;* ⁵*Department of Medicine, University of Washington, Seattle, WA;* ⁶*Statistical Center for HIV/AIDS Research and Pre, Seattle, WA;* ⁷*San Francisco Department of Public Health, San Francisco, CA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
TARGETED QUANTIFICATION OF PROTEINS AND POST-TRANSLATIONAL MODIFICATIONS**

**Yishai Levin (Weizmann Institute of Science), presiding
Ballroom III, level 4**

WOG pm 2:30 **Going Wide with Targeted Quantification of PTMs: Proteomic Connectivity Maps of Drugs, Disease, Genomics, and Beyond;** Jacob D. Jaffe; Jennifer Abelin; Jinal Patel; Jordan Taylor; Lola Fagbami; Amanda Creech; Caitlin Feeney; Xiaodong Lu; Roger Hu; Aravind Subramanian; Steven A. Carr; *The Broad Institute, Cambridge, MA*

WOG pm 2:50 **High Sensitivity Targeted Quantification of ERK Phosphorylation Dynamics and Stoichiometry without Affinity Enrichment;** Tujin Shi; Tao Liu; Matthew Gaffrey; Yuqian Gao; William Chrisler; Thomas Fillmore; Carrie Nicora; Marina Gritsenko; Chaochao Wu; Jintang He; Jia Guo; Rui Zhao; Ronald Moore; Richard Smith; David Camp, II; Karin Rodland; Steven Wiley; Wei-Jun Qian; *Pacific Northwest National Laboratory, Richland, WA*

WOG pm 3:10 **Development of a Novel 2D LC/MRM-MS Approach for Deeper and Broader Quantitation of Putative Protein Biomarkers in Human Plasma;** Romain Simon¹; Andrew Percy¹; Andrew Chambers¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada;* ²*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*

WOG pm 3:30 **Targeted Quantitation of Post-Translational Modifications and Protein-Protein Interactions of Human Nitric Oxide Synthase 2 in Airway Epithelial Cells;** Erik J Soderblom; J. Will Thompson; Kurren Mehta; Loretta G. Que; Harvey E. Marshall; M. Arthur Moseley; Matthew W. Foster; *Duke University Medical Center, Durham, NC*

WOG pm 3:50 **A Multiplex PRM Assay for Assessing Regulatory Mechanisms of Cell Death in Breast Cancer Xenografts;** Matthew R. Meyer¹; John A. Wrobel³; Kelly V. Ruggles²; Petra Erdmann-Gilmore¹; Robert Kitchens¹; Jacqueline Snider¹; Jeremy Hoog¹; Shunqiang Li¹; Sherri R. Davies¹; Matthew J. Ellis¹; David Fenyo²; R. Reid Townsend¹; ¹*Washington University in St. Louis, St. Louis, MO;* ²*New York University, New York, NY;* ³*University of North Carolina, Chapel Hill, NC*

WOG pm 4:10 **Rapid Processing of Large Scale Quantitative Proteomics Projects: Integration of Skyline with the CHORUS Cloud;** Brendan MacLean¹; Andrey Bondarenko²; Nick Shulman¹; Oleksii Tymchenko³; Christine Wu²; Nathan Yates⁴; Michael J. Maccoss¹; ¹*Univ of Washington, Seattle, WA;* ²*Stratus Biosciences, Seattle, WA;* ³*TeamDev, Kharkov, Ukraine;* ⁴*University of Pittsburgh, Pittsburgh, PA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MEMBRANE PROTEINS**

**Stephen Eyles (University of Massachusetts-Amherst), presiding
Ballroom IV, level 4**

WOH pm 2:30 **Applications of Mass Spectrometry-based Strategies for Structural Studies of 7-Transmembrane Receptors and other Membrane Proteins;** Graham M West; Bruce Pascal; Michael Chalmers; Pat Griffin; *The Scripps Research Institute, Scripps Florida, Jupiter, FL*

WOH pm 2:50 **Probing the Membrane Protein Interaction Network of *Pseudomonas aeruginosa* Cells by Chemical Cross-Linking Mass Spectrometry;** Arti Navare; Richard Siehnel; Kirsten Beck; Alejandro Wolf-Yadlin; Pradeep Singh; James E. Bruce; *University of Washington, Seattle, WA*

WOH pm 3:10 **Amphipols Outperform Detergents in the Stabilization of Membrane Protein Structure in the Gas Phase;** Antonio N. Calabrese; Tom G. Watkinson; Peter J. F. Henderson; Sheena E. Radford; Alison E. Ashcroft; *University of Leeds, Leeds, UK*

WOH pm 3:30 **The Fragmentation of Gaseous Integral Membrane Proteins;** Owen Skinner; Adam Catherman; Bryan Early; Paul Thomas; Philip Compton; Neil L. Kelleher; *Northwestern University, Evanston, IL*

WOH pm 3:50 **The Release of Membrane Protein from Detergent Micelles in the Gas Phase – Mechanistic Insights and New Detergents;** Idlir Liko; Eamonn Reading; Timothy Allison; Arthur Laganowsky; Carol V. Robinson; *University of Oxford, Oxford, Oxfordshire*

WOH pm 4:10 **Exosome Surface Proteins: Enrichment and Identification by Mass Spectrometry;** Rebecca Rose¹; Nathan Edwards³; Suzanne Ostrand-Rosenberg²; Catherine Fenselau¹; ¹*University of Maryland, College Park, MD;* ²*University of Maryland, Baltimore County, MD;* ³*Georgetown University, Georgetown, Washington, D.C.*

4:45 – 5:30 PM, WEDNESDAY AFTERNOON
ASMS MEETING

Susan T. Weintraub, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Ballroom I, level 4

5:45 – 7:00 PM, WEDNESDAY AFTERNOON
WORKSHOPS
Level 3

Light refreshments, level 3

1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Room 307-308
2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Room 309-310
3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Room 314-317
4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Room 336
5. Have Quadrupole Ion Traps Passed their Prime Time (organized by Ion Trap Interest Group); Room 337
6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Room 338
7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Room 339-340
8. Using Mass Spectrometry to Characterize the Exosome and Its Impact on Human Health; Room 341-342
9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message; Room 343-344
10. Quantitative Glycomics; Room 345-346
11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS; Nalini Sadagopan, Room 347-348
12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS (organized by Flavor Fragrance and Foodstuff Interest Group); Room 349-350
13. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History; Room 327

AFTER 8:00 PM, WEDNESDAY EVENING
CORPORATE HOSPITALITY SUITES
Hilton Hotel

THURSDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, THURSDAY MORNING
FORENSIC APPLICATIONS

Lisa Jones (Indiana Univ.-Purdue Univ. Indianapolis), presiding
Exhibit Hall AB

- ThOA am 08:30 **Qualitative Analysis of Commercially Available Household and Agrochemicals using Miniature Mass Spectrometry Coupled with Ambient Ionization**; Christopher Pulliam; Ryan Bain; Graham Cooks; *Purdue University, West Lafayette, IN*
- ThOA am 08:50 **Simultaneous Measurement of Creatinine and 11-nor-9-Carboxy-THC in Urine by Paper Spray-Mass Spectrometry for Illicit Drug Screening**; Nicholas Manicke; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- ThOA am 09:10 **Development of Hand Portable GC/MS for Onsite Arson Investigation and Screening for Toxic Chemicals on Firefighter PPE Gear**; Andrew Byrnes¹; John DeHaan²; David Matthew³; Nickesha Chung⁴; Ed Kissel⁴; Andy Saksa⁴; Eric Diken⁴; Gareth Dobson⁴; ¹Utah Valley University Emergency Services, Orem, UT; ²Fire-Ex Forensics, Vallejo, CA; ³Fire Service Consulting, Napa, CA; ⁴Smiths Detection, Danbury, CT
- ThOA am 09:30 **Direct Identification of ANFO Explosive on Real Crime Scene Samples: Banknotes and ATM Explosion Residues**; Vinicius Veri¹; Jandyson Machado¹; Jose Perez¹; Marcos Franco¹; Rodrigo Borges²; Wanderley Souza²; Jorge Zacca³; Deleon Correa⁴; Marcos Eberlin¹; ¹University of Campinas - Unicamp, Campinas, Brazil; ²Inmetro, Rio de Janeiro, Brazil; ³Brazilian Federal Police, Brasília, Brazil; ⁴Technical-Scientific Police Superintendency, São Paulo, Brazil
- ThOA am 09:50 **A Novel Forensic Approach towards Determining Time of Death Utilizing Saliva Glycosylation**; Bum Jin Kim¹; Chanyoung Han¹; Jong-Soon Choi²; Hyun Joo An¹; ¹GRAST, Chungnam National University, Daejeon, Korea; ²Korea Basic Science Institute, Daejeon, Korea
- ThOA am 10:10 **Analysis of Phenethylamine Street Drugs for Psychoactive Compounds and Impurities**; Maura McGonigal¹; Noelle Elliott²; Philip Smith¹; Frank Dorman¹; ¹Penn State, University Park, PA; ²Perkin Elmer, Shelton, CT
- 8:30 – 10:30 AM, THURSDAY MORNING
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Michael Bereman (North Carolina State University), presiding
Room 307-308
- ThOB am 08:30 **Controlled-Resonant Surface Tapping-Mode Scanning Probe Electro Spray Ionization Mass Spectrometry Imaging**; Matthias Lorenz; Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThOB am 08:50 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Mass Spectrometry for Quantification of Organobromines**; Ninghang Lin¹; Haopeng Wang¹; Kaveh Kahen²; Hamid Badiei²; Kaveh Jorabchi¹; ¹Georgetown Univ., Washington, DC; ²PerkinElmer Inc., Woodbridge, Canada
- ThOB am 09:10 **Metabolic Profiling of Single Arabidopsis Cells by Capillary Microsampling and ESI Mass Spectrometry with Ion Mobility Separation**; Linwen Zhang¹; Daniel P. Foreman¹; Paaqua A. Grant¹; Bindesh Shrestha¹; Sally A. Moody¹; Florent Villiers²; June M. Kwak^{2,3}; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²Maryland University, College Park, MD; ³Institute for Basic Science, Daegu, Republic of Korea
- ThOB am 09:30 **DMSO Enhances Electrospray Response and Boosts Sensitivity of Proteomic Experiments – Lessons Learnt from a Variety of Mass Spectrometers**; Hannes Hahne; Fiona Pachl; Benjamin Ruprecht; Susan Klaeger; Dominic Helm; Heiner Koch; Bernhard Kuster; *Technische Universität München, Freising, Germany*

ThOB am 09:50 **Development of Rapid Bedside Diagnosis Tool by Coupling of Bio-Compatible Solid Phase Microextraction (SPME) Devices to Mass Spectrometry**; German Augusto Gómez-Ríos; Barbara Bojko; Fatemeh Mirnaghi; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*

ThOB am 10:10 **Rectangular Ion Funnel (RIF): Conceptualization and Analytical Performance of a New ESI-MS Interface for Structures for Lossless Ion Manipulations (SLIM)**; Tsung-Chi Chen; Ian Webb; Marques Harrer; Spencer Prost; Sandilya Garimella; Xinyu Zhang; Jonathan Cox; Randy Norheim; Brian Lamarche; Erin Baker; Aleksey Tolmachev; Gordon Anderson; Keqi Tang; Yehia Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*

**8:30 – 10:30 AM, THURSDAY MORNING
FAIMS AND DMS: NEW DEVELOPMENTS AND APPLICATIONS
Randy Purves (University of Saskatchewan), presiding
Room 309-310**

ThOC am 08:30 **Improved Detection of SUMOylated Peptides in Large Scale Proteomic Analyses using High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS)**; Eric Bonnell; Frederic Lamoliatte; Pierre Thibault; *Université de Montréal, Montréal, QC*

ThOC am 08:50 **Differential Mobility Spectrometry of Derivatized Steroid Hormones: Examining the Relationships between Structures and Solvation**; Chang Liu¹; J. Larry Campbell¹; J.C. Yves Leblanc¹; Subhakar N. Dey²; Subhasish Purkayastha²; Tim L. Hoffman¹; ¹AB SCIEX, Concord, ON, Canada; ²AB SCIEX, Framingham, MA

ThOC am 09:10 **Fast Separation of Hydroxytestosterone Isomers using Chip-Based FAIMS Combined with Mass Spectrometry for High-Throughput Drug Assays**; Robert Smith¹; Dora Santos²; Yongmin Li²; Weichao Chen²; Kari Schlicht³; Danielle Toutoungi¹; Colin Creaser⁴; Sam Sperry⁵; ¹Owlstone Ltd, Cambridge, UK; ²Vertex Pharmaceuticals Incorporated, San Diego, CA; ³Agilent Technologies Inc, Wakefield, MA; ⁴Loughborough University, Loughborough, UK; ⁵Effector Therapeutics, San Diego, CA

ThOC am 09:30 **Improvement in the Detection of Leukemia Antigens with Differential Ion Mobility Spectrometry Coupled to Tandem Mass Spectrometry**; Samantha Isenberg; Udara Dharmasiri; Paul Armistead; Gary Glish; *University of North Carolina, Chapel Hill, NC*

ThOC am 09:50 **High Throughput Analysis using Guard-Column UHPLC-DMS-MS/MS to screen Veterinary Drug Residues in Animal Tissues**; Steven Lehotay¹; Alan Lightfield¹; Marilyn Schneider¹; Paul C. Winkler²; ¹USDA ARS, Wyndmoor, PA; ²AB Sciex, Golden, CO

ThOC am 10:10 **Evaluation of Two FAIMS Configurations for Improved Speed, Selectivity, and Sensitivity in Targeted Peptide Quantitation**; Susan E. Abbatiello; Lindsay Pino; Steven A. Carr; *The Broad Institute of MIT and Harvard, Cambridge, MA*

**8:30 – 10:30 AM, THURSDAY MORNING
RADICAL ION CHEMISTRY**

**Benjamin Bythell (University of Missouri-St. Louis), presiding
Room 314-317**

ThOD am 08:30 **Kinetic Ion Thermometers (KIT) for the Determination of Internal Energy in Transient Peptide Cation-Radicals Formed by Electron Transfer**; Frantisek Turecek; Robert Pepin; *University of Washington, Seattle, WA*

ThOD am 08:50 **Formation and Reaction of Methoxy Radical with Disulfide Linked Peptides in a NanoESI Plume: Chemistry and Utility**; Kirt L. Durand; Craig Stinson; Xiaoxiao Ma; Chasity Love; Yu Xia; *Purdue University, West Lafayette, IN*

ThOD am 09:10 **“How Sweet It Is”: Development of a New Method for Generating Sugar Radical Cations via Non-Covalent Complexes**; Sandra Osburn; Spencer J. Williams; Richard A.J. O’Hair; *University of Melbourne, Parkville, Australia*

ThOD am 09:30 **Radical Delivery and Radical Fragmentation with Crown Ether Attachment for Structural Analysis of Biomolecules**; Huong T (Nicole) Pham; Ryan R. Julian; *University of California, Riverside, CA*

ThOD am 09:50 **Identification of the Presence of Isomeric Reactant Ions Based on their Ion-Molecule Reaction Kinetics**; Ashley Wittrig; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*

ThOD am 10:10 **Tuning Radical Reactivity by Polarity Switching in Gas Phase Distonic Ions**; David Marshall²; Lifu Ma²; Benjamin Kirk³; Adam Trevitt²; Stephen J Blanksby¹; ¹Queensland University of Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia; ³Lawrence Berkeley National Laboratory, Berkeley, CA

**8:30 – 10:30 AM, THURSDAY MORNING
BIOMARKERS IN DRUG DISCOVERY,
DEVELOPMENT AND DIAGNOSIS
Nathalie Agar (Harvard Medical Center), presiding
Ballroom I, level 4**

ThOE am 08:30 **Identification of Translational Biomarkers in Drug Discovery: Animal Model Optimization and Experimental Design**; Petia Shipkova; Joelle Onorato; Dong Cheng; Anthony Azzara; Don Robertson; *Bristol Myers Squibb, Princeton, NJ*

ThOE am 08:50 **Rapid Assessment of Apoptotic Signaling to Study Synergy of Cancer Chemotherapeutics**; Robert Sprung¹; Mark Meads¹; Luis Saavedra-Roman²; Elizabeth Wood¹; Wei Guan¹; David Britton³; Ian Pike³; Kenneth Shain¹; John Koomen¹; ¹H. Lee Moffitt Cancer Center, Tampa, FL; ²University of South Florida, Tampa, FL; ³Proteome Sciences, London, UK

ThOE am 09:10 **Tracer Methodologies for Measuring Triglyceride Metabolism in Pharmaceutical Research & Development: How to Get the Skinny on Fat**; David McLaren; Steven Stout; Dan Xie; Ying Chen; Seongah Han; Jinqi Liu; Sheng-Ping Wang; Raymond Rosa; Vivienne Mendoza; Olga Berejnaia; Gowri Bhat; Paul Miller; Pan Yi; Kithsiri Herath; Ablatt Mahsut; Vinit Shah; Dunlu Chen; Beth Ann Murphy; Karen Akinsanya; Hayes Dansky; Jose Castro-Perez; Shirlly Pinto; Douglas Johns; Stephen Previs; Thomas Roddy; *Merck & Co., Inc., Kenilworth, NJ*

- ThOE am 09:30 **Understanding Uptake and Trafficking Pathways Taken by Liver-Targeted siRNAs by Looking for Metabolite Breadcrumbs using High Resolution Mass Spectrometry**; Christopher Kochansky; Kristen Kwasnjuk; Michael Lyman; BaoJen Shyong; Kristin Geddes; Heather Trexler; Charles Thompson; Mark Cancilla; *Merck Research Labs, West Point, PA*
- ThOE am 09:50 **Serum Protein Biomarkers to Monitor Duchenne Muscular Dystrophy Disease Progression and Response to Therapy**; Ramya L Marathi¹; Sree Rayavarapu¹; Aiping Zhang¹; Haeri Seol¹; Kristy J Brown¹; Heather Gordish-Dressman¹; Kanneboyina Nagaraju¹; Eric P Hoffman¹; Erik Henricson²; Craig McDonald²; Yerib Houthout¹; ¹*Children's National Medical Center, Washington D.C., DC*; ²*University of California, Davis School of Medicine, Davis, CA*
- ThOE am 10:10 **Integrated Analysis of Proteomic and Genomic Data from Breast Cancer Tumor Profiles**; D. R. Mani¹; Philipp Mertins¹; Pei Wang^{2,3}; Karl R. Clauser¹; Michael A. Gillette¹; Jana W. Qiao¹; Xianglong Wang²; Yuzheng Zhang²; Ping Yan²; Chenwei Lin²; Amanda Paulovich²; Steven A. Carr¹; ¹*Broad Institute of MIT and Harvard, Cambridge, MA*; ²*Fred Hutchinson Cancer Research Center, Seattle, WA*; ³*Mount Sinai School of Medicine, New York, NY*
- 8:30 – 10:30 AM, THURSDAY MORNING
COVALENT LABELING, CHEMICAL PROBES, AND
CROSSLINKING FOR BIOMOLECULE
STRUCTURAL CHARACTERIZATION**
**Simin Maleknia (University of New South Wales), presiding
Ballroom II, level 4**
- ThOF am 08:30 **Extending the Cross-Linking/MS Strategy: Monitoring Protein Conformations by Incorporation of Unnatural Amino Acids, Photo-Cross-Linking, and MS**; Rico Schwarz; Knut Koelbel; Philip Loessl; Christian Ihling; Andrea Sinz; *Martin Luther University Halle, Halle, Germany*
- ThOF am 08:50 **Structural Characterization using Chemical Cross-linking and Hydrogen/Deuterium Exchange: Resource for Novel Model of Human Haptoglobin**; Zdenek Kukacka^{1,2}; Petr Man^{1,2}; Petr Novak^{1,2}; Petr Pompach^{1,2}; ¹*Institute of Microbiology ASCR, Prague, Czech Republic*; ²*Faculty of Science, Charles University, Prague, Czech Republic*
- ThOF am 09:10 **A Novel Bioorthogonal and Clickable Cross-Linker for improved Protein/Protein Interaction Analysis**; Catherine Nury^{1,2}; Virginie Redeker³; Sébastien Dautry⁴; Anthony Romieu⁴; Guillaume Van der Rest⁵; Pierre-Yves Renard⁴; Ronald Melki³; Julia Chamot-Rooke^{1,2}; ¹*CNRS UMR 3528, Institut Pasteur, Paris, France, Paris, France*; ²*Institut Pasteur, Structural MS & Proteomics Unit, Paris, France*; ³*Laboratoire Enzymologie et Biochimie Structurales, Gif sur Yvette, France*; ⁴*Université de Rouen - UMR 6014 CNRS, Mont Saint Aignan, France*; ⁵*Université Paris Sud, Lab. Chimie Physique, Orsay, France*
- ThOF am 09:30 **Mass-Spectrometry-Based Footprinting to Map the Precursor tRNA Binding Sites in a Protein-Only RNase P Variant**; Tien-Hao Chen; Akiko Tanimoto; Xin Ma; Wei Zhou; Jikang Wu; Venkat Gopalan; Vicki Wysocki; *The Ohio State University, Columbus, OH*
- ThOF am 09:50 **High Resolution Measurement of Protein Topography by Covalent Carbene Labeling Induced by Single-Shot Laser Irradiation**; Joshua Buse¹; Ryan Bomgardner²; John Rogers²; Chris Etienne²; David C. Schriemer¹; ¹*University of Calgary, Calgary, Alberta*; ²*Thermo Fisher Scientific, Rockford, Illinois*
- ThOF am 10:10 **Probing the Conformational Change of Orange Carotenoid Protein during Photo-Activation in Cyanobacteria**; Hao Zhang; Haijun Liu; Jeremy King; Mindy Prado; Michael L. Gross; Robert E. Blankenship; *Washington University, St Louis, MO*
- 8:30 – 10:30 AM, THURSDAY MORNING
INFORMATICS: METABOLOMICS**
**Pieter Dorrestein (University of California, San Diego), presiding
Ballroom III, level 4**
- ThOG am 08:30 **Searching PubChem with Tandem Mass Spectrometry Data: Teaming Molecular Fingerprint Prediction and Fragmentation Trees**; Sebastian Böcker¹; Huibin Shen²; Kai Dührkop¹; Juho Rousu²; ¹*Friedrich-Schiller-University Jena, Jena, Germany*; ²*Aalto University, Helsinki, Finland*
- ThOG am 08:50 **ramclustR: post-XCMS Feature Clustering for Data Reduction and Spectral Matching-Based Annotation**; Corey Broeckling¹; Fayyaz-ul-Amir Afsar Minhas¹; Asa Ben-Hur¹; Jessica Prenni¹; Steffen Neumann²; ¹*Colorado State University, Fort Collins, CO*; ²*Leibniz Institute of Plant Biochemistry, Halle, Germany*
- ThOG am 09:10 **Multivariate Analysis, Visualization and Network Tools for Biological Interpretation of Metabolomic Data**; Dmitry Grapov^{1,2}; Oliver Fiehn^{1,2}; ¹*NIH West Coast Metabolomics Center, Davis, CA*; ²*University of California, Davis, Davis, CA*
- ThOG am 09:30 **Database Driven Molecular Annotation of Imaging Mass Spectrometry**; Andrew D. Palmer¹; Michael Becker²; Janina Oetjen³; Ilya Chernyavsky¹; Dmitry N. Kozlov¹; Theodore Alexandrov^{1,4}; ¹*University of Bremen, Bremen, Germany*; ²*Bruker Daltonik GmbH, Bremen, Germany*; ³*MALDI Imaging Lab, University of Bremen, Bremen, Germany*; ⁴*SCiLS GmbH, Bremen, Germany*
- ThOG am 09:50 **Mass Spectrometry Based Metabolomics Work Area and Data Management Software "From Sample to Metabolic Pathways"**; Bernd Haas; Martin Buratti; Nicole Huber; Hannes Pedevilla; Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Österreich*
- ThOG am 10:10 **Lifeline-S.O.S: "Crowd Curation" of Unidentified GC-(EI)MS spectra through Social Online Spectrometry**; Manor Askenazi¹; Yuri Mirokhin²; Stephen Stein²; ¹*Biomedical Hosting LLC, Arlington, MA*; ²*NIST, Gaithersburg, MD*
- 8:30 – 10:30 AM, THURSDAY MORNING
GLYCOPROTEINS AND GLYCANS: NEW MS APPROACHES**
**Ronghu Wu (Georgia Tech), presiding
Ballroom IV, level 4**
- ThOH am 08:30 **Determination of the False Discovery Rate in Glycopeptide Identifications using GlycoPep Evaluator**; Zhikai Zhu; Xiaomeng Su; Eden Go; Heather Desaire; *University of Kansas, Lawrence, KS*

THURSDAY MORNING AND THURSDAY AFTERNOON ORAL SESSIONS

ThOH am 08:50 **Method for Analysis of Glycan Degradation Products in the Feces of Breast-Fed Newborns;** Jasmine C. C. Davis; Sarah M. Totten; Carlito B. Lebrilla; *UC Davis, Davis, CA*

ThOH am 09:10 **Relative Quantification of Glycans using Multiplexed Carbonyl-Reactive Tandem Mass Tags and CE-ESI-MS;** Xuefei Zhong¹; Yan Liu²; Sergei Snovida³; John Rogers³; Lingjun Li¹; ¹*University of Wisconsin Madison, Madison, WI*; ²*Xiamen University, Xiamen, P.R.China*; ³*Thermo Fisher Scientific, Rockford, IL*

ThOH am 09:30 **Stable Isotope Labeling Strategies for Quantitative UPLC-MS Based Glycomics;** Silvia Millan Martin¹; Simone Albrecht¹; Margaret Doherty¹; Cedric Delporte¹; Niaobh McLoughlin¹; Natalia Navas²; Jonathan Bones¹; ¹*NIBRT, Dublin, Ireland*; ²*University of Granada, Granada, Spain*

ThOH am 09:50 **Quantitative LC-MS/MS Glycomic Analysis using Tandem Mass Tag (TMT);** Shiyue Zhou¹; Yunli Hu¹; Sergei Snovida²; John C. Rogers²; Julian Saba³; Yehia Mechref¹; ¹*Texas Tech University, Lubbock, TX*; ²*Thermo Fisher Scientific, Rockford, IL*; ³*Thermo Fisher Scientific, San Jose, CA*

ThOH am 10:10 **A Novel Method for Quantitative Analysis of Sialylated Glycopeptides;** Punit Shah; Shadi Toghi Eshghi; Weiming Yang; Jing Chen; Lijun Chen; Hui Zhang; *Johns Hopkins University School of Medicine, Baltimore, MD*

10:30 AM – 2:30 PM, THURSDAY
THURSDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm

THURSDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, THURSDAY AFTERNOON FOOD CHEMISTRY AND SAFETY Clifton K. Fagerquist (USDA), presiding Exhibit Hall AB

ThOA pm 2:30 **Integrated Targeted and Untargeted Analysis of Ergot Alkaloids in Cereals using UHPLC – TripleTOF MS;** José Diana Di Mavungu; Sarah De Saeger; *Ghent University, Ghent, Belgium*

ThOA pm 2:50 **The Molecular Architecture of an Edible Biofilm;** Laura Sanchez¹; Julie Button²; Theodore Alexandrov³; Benjamin Wolfe²; Rachel Dutton²; Pieter Dorrestein¹; ¹*University of California, San Diego, Skaggs school, La Jolla, CA*; ²*Harvard FAS Center for Systems Biology, Cambridge, MA*; ³*University of Bremen, Bremen, Germany*

ThOA pm 3:10 **Ion Mobility Studies of Isomeric Species Lycopene, β -carotene, and α -carotene and the Retention of Trans and Cis Conformation;** Matthew Bernier; Rachel Kopec; Steven Schwartz; Vicki Wysocki; *The Ohio State University, Columbus, OH*

ThOA pm 3:30 **Simultaneous Quantitative Determination of Melamine, Ammeline, Ammelide, Cyanuric acid and Dicyandiamide in Infant Formula and Other Foods by UHPLC-MS/MS with Fast Polarity Switching;** Hui Zhao; Katerina Mastovska; James Stark; Brent Rozema; John Austad; *Covance, Madison, WI*

ThOA pm 3:50 **Evaluating *terroir* - Revealing the Chemical Basis of Organoleptic Properties of Cabernet Sauvignon Wine with Untargeted LC and GC/QTOF Workflows;** Stephan Baumann¹; Susan Ebeler²; Frank David³; Mark Sartain¹; Sofia Aronova¹; Kawaljit Tandon⁴; ¹*Agilent Technologies, Inc., Santa Clara, CA*; ²*UC Davis Department of Viticulture and Enology, Davis, CA*; ³*Research Institute for Chromatography, Kortrijk, Belgium*; ⁴*Constellation Brands, Inc., Madera, CA*

ThOA pm 4:10 **Application of Wheat-Specific Peptide Markers for the Detection of Gluten in an incurred Cornbread Model using Mass Spectrometry;** Katherine L. Fiedler¹; Sara C. McGrath¹; Lauren S. Jackson²; Mark M. Ross¹; ¹*U.S. FDA, CSFAN, College Park, MD*; ²*U.S. FDA, CFSAN, Bedford Park, IL*

2:30 – 4:30 PM, THURSDAY AFTERNOON INSTRUMENTATION: TIME-OF-FLIGHT MASS SPECTROMETRY William Brinckerhoff (NASA), presiding Room 307-308

ThOB pm 2:30 **Space- and Time-Resolved Detection of Ions and Neutrals in MALDI-TOF-MS Using an Active Pixel Detector;** Shane R. Ellis; Ron M.A. Heeren; *FOM Institute AMOLF, Amsterdam, Netherlands*

ThOB pm 2:50 **MALDI-TOF-MS-Analysis of Intact High Mass Proteins by Phonon-Assisted Field Emission in Silicon Nanomembranes;** Diana Hildebrand¹; Hyun-Cheol Shin Shin^{1,2}; Hyunseok Kim Kim²; Jonghoo Park³; Zlatan Aksamija Aksamija⁴; Robert Blick^{1,2}; ¹*University of Hamburg, Hamburg, Germany*; ²*University of Wisconsin-Madison, Madison, WI*; ³*Kyungpook National University, Daegu, Korea*; ⁴*University of Massachusetts-Amherst, Amherst, MA*

ThOB pm 3:10 **High Resolution Multi-Reflecting TOFMS with Ion Trap Converter;** Vlatcheslav Artaev¹; Sergey Kirillov²; Boris Kozlov²; Mikhail Yavor²; Anatoly Verenchikov²; ¹*LECO Corporation, St Joseph, MI*; ²*Mass Spectrometry Consulting, Bar, Montenegro*

ThOB pm 3:30 **Instrumentation, Statistics and Inference in TOFMS;** Andreas Ipsen; *Swansea University, Swansea, UK*

ThOB pm 3:50 **Perfect Timing: Fragment Ion Mobility Based Performance Increase on a qTOF Instrument;** Dominic Helm¹; Christopher J Hughes²; Johannes PC Vissers²; Benjamin Ruprecht¹; Hannes Hahne¹; Isabelle Becher³; Markus Bantscheff³; James I Langridge²; Bernhard Kuster¹; ¹*Technische*

Universität München, Freising, Germany; ²Waters Corporation, Manchester, UK; ³Cellzome, Heidelberg, Germany

- ThOB pm 4:10 **Transient Sample Introduction with Laser Ablation Coupled to an Inductively Coupled Plasma Distance-of-Flight Mass Spectrometer (ICP-DOFMS);** Elise A. Dennis¹; Alexander W. Gundlach-Graham¹; Christie G. Enke²; Steven J. Ray¹; Charles J. Barinaga³; David W. Koppenaal³; Gary M. Hieftje¹; ¹Indiana University, Bloomington, IN; ²University of New Mexico, Placitas, NM; ³Pacific Northwest National Laboratory, Richland, WA

**2:30 – 4:30 PM, THURSDAY AFTERNOON
MASS SPECTROMETRY IN STRUCTURAL BIOLOGY
Christian Bleiholder (Florida State University), presiding
Room 309-310**

- ThOC pm 2:30 **Integrating Native Mass Spectrometry with (Quantitative) Proteomics and Comparative Chemical Cross-linking – Insights into the Assembly of Key Protein Complexes;** Carla Schmidt; Yuliya Gordiyenko; Nina Morgner; Min Zhou; Carol Robinson; *University of Oxford, Oxford, UK*
- ThOC pm 2:50 **Using Surface Induced Dissociation-Ion Mobility (SID-IM) to Distinguish the Different Interfaces that Exist in Tetrameric Protein Complexes;** Royston Quintyn; Jing Yan; Vicki Wysocki; *The Ohio State University, Columbus, Ohio*

- ThOC pm 3:10 **Metabolic Pulse Chase Labeling of Rodents Shows that the Protein Cores of Some Intracellular Protein Machines Last a Lifetime;** Jeffrey Savas¹; Brandon Toyama²; Varda Levram-Ellisman³; Roger Tsien³; Martin Hetzer²; John Yates¹; ¹The Scripps Research Institute, La Jolla, CA; ²Salk Institute for Biological Studies, La Jolla, CA; ³University of California at San Diego, La Jolla, CA

- ThOC pm 3:30 **Charge Detection Mass Spectrometry Measures Mass Distribution of Virus Capsids above 20 MDa and Resolves Intermediates in Virus Assembly;** David Keifer; *Indiana University, Bloomington, IN*

- ThOC pm 3:50 **Large Scale Protein-Protein Complex Structure Prediction with *in vivo* Cross-Linking Data;** Chunxiang Zheng; Juan Chavez; Arti Navare; Xia Wu; James Bruce; *University of Washington, Seattle, WA*

- ThOC pm 4:10 **Droplet Sizes, Electrospray Currents, and Nonspecific Aggregation in Electrokinetically Controlled Native Nanoelectrospray Ionization;** Kimberly Davidson¹; Derek Oberreit²; Christopher Hogan²; Matthew Bush¹; ¹University of Washington, Seattle, WA; ²University of Minnesota, Minneapolis, MN

**2:30 – 4:30 PM, THURSDAY AFTERNOON
FUNDAMENTALS: ION SPECTROSCOPY
Elaine Marzluff (Grinnell College), presiding
Room 314-317**

- ThOD pm 2:30 **Fluorescence Resonance Energy Transfer Measurements for the Structural Characterization of Gaseous Proteins Generated by Electrospray Ionization;** Martin F. Czar¹; Arash Zarrine-Afsar²; Franziska Zosel²; Iwo König²; Benjamin Schuler²; Rebecca A. Jockusch¹; ¹University of Toronto, Toronto, Canada; ²Universität Zürich, Zürich, Switzerland

- ThOD pm 2:50 **Action-EET Based Dissociation of Disulfide Bonds with Tryptophan as a Donor in the Gas Phase;** Nathan Hendricks¹; Nichole M. Lareau²; John A. Mclean²; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA; ²Vanderbilt University, Nashville, TN

- ThOD pm 3:10 **Conformer-Specific Infrared Spectroscopy of Cyclic b_6 and b_8 Fragments Produced by Collision-Induced Dissociation of Peptides;** Oleg Aseev; Marta Perez; Ursula Röthlisberger; Thomas Rizzo; *École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

- ThOD pm 3:30 **Gas-phase Conformation of Polyproline Peptides and the b_2 Fragment by IRMPD Spectroscopy;** Jonathan Martens¹; Josipa Grzetic¹; Giel Berden¹; Jos Oomens^{1,2}; ¹Radboud University Nijmegen, Nijmegen, Netherlands; ²University of Amsterdam, Amsterdam, Netherlands

- ThOD pm 3:50 **Infrared Multiple Photon Dissociation Spectroscopy of a Gas-Phase Oxo-Molybdenum Complex with 1,2-dithiolene Ligands;** Michael J. Van Stipdonk¹; John K. Gibson²; Giel Berden³; Jos Oomens^{3,4}; ¹Duquesne University, Pittsburgh, PA; ²Lawrence Berkeley Laboratory, Berkeley, CA; ³Radboud University Nijmegen, Nijmegen, The Netherlands; ⁴University of Amsterdam, Amsterdam, The Netherlands

- ThOD pm 4:10 **Soft Landing of Mass-Selected Polyoxometalate Anions onto Self-Assembled Monolayers;** Don Gunaratne; Grant Johnson; Amity Andersen; Dan Du; Weiyang Zhang; Yuehe Lin; Julia Laskin; *Pacific Northwest National Laboratory, Richland, WA*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
DATA INDEPENDENT ACQUISITION
Paul West (Biomarker Discovery), presiding
Ballroom I, level 4**

- ThOE pm 2:30 **Comparison of Shotgun Proteomics with Data Independent Acquisition in Terms of Number of Identified Peptides;** Roland M. Bruderer; Oliver M. Bernhardt; Saša M. Miladinović; Tejas Gandhi; Oliver Rinner; Lukas Reiter; *BiognoSYS AG, Zurich, Switzerland*

- ThOE pm 2:50 **Multiphase-cHiPLC Coupled SWATH Profiling of Metastatic Melanoma Cells Reveals MAPK Pathway Mutation Specific Protein Expression;** Christoph Krisp¹; Robert Parker¹; Matthew McKay¹; Dana Pascovici¹; Hao Yang²; Remco van Soest²; Tina Settineri²; Mark P. Molloy¹; ¹Australian Proteome Analysis Facility, Sydney, Australia; ²Eksigent, part of AB SCIEX, Redwood City, CA

- ThOE pm 3:10 **Systematic Investigation on Suitability of LC-QqTOF with SWATH Acquisition for Routine Forensic Screenings-Comparison with IDA and Targeted MRM Approaches;** Andreas T. Roemmel; Andrea E. Steuer; Michael Poetzsch; Thomas Kraemer; *Zurich Institute of Forensic Medicine, UZH, Zurich, Switzerland*

ThOE pm 3:30 **Harnessing the Power of SWATH-MS for Unbiased Identification of O-GlcNacetylated Proteins;** Christine Jelinek; Genaro Ramirez-Correa; Guanghui Han; David Colquhoun; Alexey Lyashkov; Gerald Hart; David Graham; Jennifer Van Eyk; Anne Murphy; *Johns Hopkins School of Medicine, Baltimore, MD*

ThOE pm 3:50 **Increasing Depth of Coverage in Data Independent Acquisition with Acquisition Improvements and Higher Sample Loads;** Christie L. Hunter¹; Ben Collins²; Ludovic Gillet²; Ruedi Aebersold²; ¹AB SCIEX, Redwood City, CA; ²ETH Zurich, Zurich, Switzerland

ThOE pm 4:10 **Establishment of DIA-based Methods in Urine Biomarker Discovery - A Comparative Study to Discover an Early Stage Chronic Pancreatitis Biomarker;** Jan Muntel¹; Saima Ahmed¹; Melena Bellin²; Vivek Kadiyala³; Shadeah L. Suleiman³; Linda S. Lee³; Peter A. Banks³; Darwin L. Conwell⁴; Hanno Steen¹; ¹Boston Children's Hospital, Boston, MA; ²University of Minnesota, Minneapolis, MN; ³Brigham and Women's Hospital, Boston, MA; ⁴Ohio State University Wexner Medical Center, Columbus, OH

**2:30 – 4:30 PM, THURSDAY AFTERNOON
EPIGENETIC MODIFICATIONS AND MECHANISMS**
Maria Person (University of Texas, Austin), presiding
Ballroom II, level 4

ThOF pm 2:30 **Stable Isotope labeled Histone Peptide Library for Histone Post-Translational Modification and Variant Quantification by Mass Spectrometry;** Shu Lin¹; Samuel Wein¹; Michelle Gonzales-Cope^{1,2}; Gabriel L. Otte¹; Leila Afjehi-Sadat¹; Tobias Maile³; Shelley L. Berger¹; John Rush⁴; Jennie Lill³; David Arnott³; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²Princeton University, Princeton, NJ; ³Genentech Inc., South San Francisco, CA; ⁴Cell Signaling Technology Inc., Danvers, MA

ThOF pm 2:50 **Differential Analysis of histone Post Translational Modifications in MEL Cells using WCX-HILIC Coupled to Middle-Down ECD Mass Spectrometry;** Annie Moradian¹; Michael Sweredoski¹; Anastasia Kalli²; Sonja Hess¹; ¹California Institute of Technology, Pasadena, CA; ²Children's Hospital Los Angeles, Los Angeles, CA

ThOF pm 3:10 **Top Down MS/MS Analysis of Dynamic Changes in Histone Sequence Variants and Post-Translational Modifications during HIV Activation;** Yu Chen¹; Xibei Dang¹; Brian D. Spetman²; Jonathan H. Dennis²; Alan G. Marshall^{1,2}; Nicolas L. Young¹; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University, Tallahassee, FL

ThOF pm 3:30 **Dynamic and Combinatorial Landscape of Histone Modifications through Plasmodium falciparum Life Cycle;** Anita Saraf¹; Serena Cervantes²; Evelien Bunnik²; Nadia Pons²; Mihaela Sardu¹; Duk-Won Chung²; Jacques Prudhomme²; Zhihui Wen¹; Joseph Varberg¹; Michael Washburn¹; Karine Le Roch²; Laurence Florens¹; ¹Stowers Institute for Medical Research, Kansas City, MO; ²University of California Riverside, Riverside, CA

ThOF pm 3:50 **Quantitative Profiling of Chromatome Dynamics Reveals the Regulatory Switches of Epigenome in Hypoxia-Induced Oncogenesis;** Bamaprasad Dutta; Siu Kwan Sze; *Nanyang Technological University, Singapore, Singapore*

ThOF pm 4:10 **Protein Profiling Reveals Dynamic H1 Expression and Identifies H3 K9me/S10p/K14ac tri-modification Forms in Monocyte Differentiation;** Hui Tang; Kangling Zhang; *University of Texas Medical Branch at Galveston, Galveston, TX*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
METABOLOMICS/LIPIDOMICS:
NEW MS TECHNOLOGIES AND APPLICATIONS**
Stephen Blanksby (Queensland University), presiding
Ballroom III, level 4

ThOG pm 2:30 **Comprehensive Lipidome Profiling Enables Functional Studies to Determine the Role of Aberrant Lipid Metabolism in Metastatic Colorectal Cancer Cells;** Cassie Phaner; Gavin E. Reid; *Michigan State University, East Lansing, MI*

ThOG pm 2:50 **Integration of Supercritical Fluid Chromatography with Ion Mobility-Mass Spectrometry (SFC-IM-MS) for Metabolomics and Lipidomics;** Rafael Montenegro Burke¹; Cody Goodwin¹; Libin Xu¹; Zeljka Korade²; Brian Bachmann¹; Ned Porter¹; John A. Mclean¹; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt Kennedy Center, Nashville, Tennessee

ThOG pm 3:10 **Applications and Performance of the GC/quadrupole-Orbitrap MS in Discovery Metabolomics;** Allison Balloun¹; Jason Cole³; Taylor Wahlig¹; Amelia Petersen²; Jens Griep-Raming²; Michael Westphal¹; Jean-Michel Ane¹; Michael Sussman¹; Joshua Coon¹; ¹University of Wisconsin, Madison, WI; ²Thermo Fisher Scientific, Bremen, Germany; ³Thermo Fisher Scientific, Austin, TX

ThOG pm 3:30 **Accurate Quantification of Polyunsaturated Glycerophospholipids by Shotgun Lipidomics;** Kai Schuhmann; Andrej Shevchenko; *MPI-CBG, Dresden, Germany*

ThOG pm 3:50 **Facile Determination of C=C Bonds within Lipids by On-Line Paternò-Büchi Reaction and Tandem Mass Spectrometry;** Xiaoxiao Ma; Yuan Su; Zheng Ouyang; Yu Xia; *Purdue University, West Lafayette, IN*

ThOG pm 4:10 **A Sensitive Mass Spectrometry Platform Providing Ozone Induced Dissociation for High Throughput Lipid Structure Characterization;** Qibin Zhang; Yehia Ibrahim; Karl Weitz; Ronald Moore; Richard D. Smith; Keqi Tang; *Pacific Northwest National Laboratory, Richland, WA*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
CARBOHYDRATES: NEW MS APPROACHES**
Maria Lorna De Leoz (NIST), presiding
Ballroom IV, level 4

ThOH pm 2:30 **Application of Selected Accumulation Ion Mobility Spectrometry-Electron Activated Dissociation Tandem Mass Spectrometry in Structural Analysis of Isomeric Glycans;** Yi Pu¹; Rebecca S. Glaskin²; Cheng Lin²; Catherine E. Costello^{1,2}; ¹Boston University, Boston, MA; ²Boston University School of Medicine, Boston, MA



ThOH pm 2:50 **Comparing the LC-MS of Permethylated and Native Glycans on Reversed-Phase and Porous Graphitic Carbon Columns;** [Yunli Hu](#); Shiyue Zhou; James Blackmer; Yehia Mechref; *Texas Tech University, Lubbock, TX*

ThOH pm 3:10 **Exploring the Brain Glycome using Tissue Cell Membrane Capture and Nanoflow Liquid Chromatography/Mass Spectrometry;** [Injung Ji](#)¹; Serenus Hua¹; Jong-Soon Choi²; Hyun Joo An¹; ¹*AGRS, Chungnam National University, Daejeon, Korea*; ²*Division of Life Science, KBSI, Daejeon, Korea*

ThOH pm 3:30 **Oligosaccharide MSn and Spectral Library Matching: Instrumental and Collision Energy Comparisons;** Andrew Hanneman¹; David Ashline^{1,2}; Hailong Zhang²; [Vernon Reinhold](#)²; ¹*Glycan Connections, Lee, NH*; ²*University of New Hampshire, Durham, NH*

ThOH pm 3:50 **Fully Automated Annotation and Identification of Glycosaminoglycan MS/MS Spectra;** [Jiana Duan](#); Jon Amster; *University of Georgia, Athens, GA*

ThOH pm 4:10 **Discovery of a Novel Peeling Reaction that Contributes to the Underestimation of 3-O-sulfation in Heparan Sulfate;** Yu Huang¹; Yang Mao¹; Chengli Zhong²; Geert-Jan Boons²; Cheng Lin¹; [Joseph Zaia](#)¹; ¹*Boston University School of Medicine, Boston, MA*; ²*University of Georgia, Athens, GA*

4:45 – 5:30 PM, THURSDAY AFTERNOON
PLENARY LECTURE
Jenny Brodbelt (University of Texas, Austin), presiding
Exhibit Hall AB



How The Genome Folds
Erez Lieberman Aiden
Baylor College of Medicine and Rice University

6:30 – 9:00 PM, THURSDAY
CLOSING EVENT
National Aquarium
Ticket is required.



7:30 – 8:00 am..... Set up all Monday posters
 10:30 am – 1:00 pm..... Odd-numbered posters present
 12:00 – 2:30 pm..... Even-numbered posters present
 7:30 – 8:00 pm..... Remove all Monday posters

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LCMS: Chromatography.....	727-752
LCMS: Sample Preparation (Drugs and Metabolites).....	753-786

These special posters will be displayed all week.

Special **The Analytical Triple-Quadrupole Mass Spectrometer and Low-Energy CID: Beginnings, Offshoots, and Current Applications;** [Michael A. Grayson](#)¹; [Christie G. Enke](#)²; [Richard A. Yost](#)³; ¹*Retired, St Charles, MO*; ²*University of New Mexico, Placitas, NM*; ³*University of Florida, Gainesville, FL*

Special **The British Mass Spectrometry Society: The first 50 years;** [Alison E. Ashcroft](#)¹; [Susan Crosland](#)²; [Keith R Jennings](#)³; ¹*University of Leeds, Leeds, United Kingdom*; ²*Syngenta, Jealott's Hill, Bracknell, UK*; ³*2 Meadow Croft Drive, Bishop Monkton, UK*

Special **Call for Participants for the iPRG 2015 Study: Label-Free Quantitative Proteomics Data Analysis**

Imaging MS: Method Development, 001 - 018

MP 001 **Systematic Study of Stage Raster Speed, Laser Repetition Rate and Pulse Energy in MALDI MSI;** [Rory T. Steven](#); [Ian S. Gilmore](#); [Josephine Bunch](#); *National Physical Laboratory, London, UK*

MP 002 **High Throughput Spatially Resolved Peptide Identification using Hydrogel Digestion and Electro-Elution;** [Erin H. Seeley](#); [Gregory Boyce](#); [Linda Prengaman](#); [Greg W. Kilby](#); *Protea Biosciences, Inc., Morgantown, WV*

MP 003 **Quality Measures of MALDI MS imaging;** [Oskar Karlsson](#); [Malin Andersson](#); *Uppsala University, Uppsala, Sweden*

MP 004 **Multicenter MALDI Mass Spectrometry Imaging Identifies Proteomic Markers of Stromal Activation in Breast Cancer;** [Tim Dekker](#)¹; [Benjamin Balluff](#)¹; [Emrys Jones](#)¹; [Cedrik Schoene](#)²; [Michaela Aubele](#)²; [Manfred Schmitt](#)³; [Judith Kroep](#)¹; [Vincent Smit](#)¹; [Rob Tollenaar](#)¹; [André Deelder](#)¹; [Wilma Mesker](#)¹; [Axel Walch](#)²; [Liam McDonnell](#)¹; ¹*Leiden University Medical Center, Leiden, Netherlands*; ²*Helmholtz Zentrum Muenchen, Munich, Germany*; ³*Klinikum rechts der Isar, Munich, Germany*

MP 005 **Imaging Mass Spectrometry and Depth Profiling for the Organic Thin Film using Laser Desorption Ionization;** [Takaya Satoh](#)¹; [Masahide Shima](#)¹; [Hironobu Niimi](#)¹; [Yoji Nakajima](#)²; [Makiko Fujii](#)³; [Toshio Seki](#)³; [Jiro Matsuo](#)³; [Robert DiPasquale](#)⁴; ¹*JEOL Ltd., Akishima, Japan*; ²*Saahi Glass Co., Ltd., Yokohama, Japan*; ³*Kyoto Univ., Kyoto, Japan*; ⁴*JEOL USA Inc., Peabody, MA*

MP 006 **Using MALDI-IMS and Membrane Microarrays for Tissue Classification;** [Roberto Fernández](#)¹; [Tarson Tolentino-Cortez](#)²; [Sergio Lage](#)³; [Jone Garate](#)¹; [Izaskun Erguido](#)¹; [Rafael Rodríguez-Puertas](#)¹; [Egoitz Astigarraga](#)²; [Gabriel Barreda-Gómez](#)²; [José A. Fernández](#)¹; ¹*University of Basque Country, Leioa, Spain*; ²*IMG Pharma Biotech, Leioa, Spain*; ³*Cruces University Hospital, Barakaldo, Spain*

MP 007 **Sensitive Imaging of Essential Elements in a Rat Cerebellum using an Optimized LA/ICP-MS Setup Including a Collision Reaction Interface;** [Rebecca Niehaus](#); [Christoph Alexander Wehe](#); [Michael Sperling](#); [Uwe Karst](#); *Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

MP 008 **In-depth Identification of Protein Images by Combining High Mass Resolution MALDI FTICR Imaging and High Performance qTOF nLC-MS/MS;** [Shannon Cornett](#); [Sergei Dikler](#); [Matt Willetts](#); *Bruker Daltonics Inc., Billerica, MA*

MP 009 **Integration and Application of Separation Strategies to Multiplex Imaging Mass Spectrometry for Complex Neuropeptide Analysis;** [Shan Jiang](#); [Zichuan Zhang](#); [Lingjun Li](#); *UW-Madison, Madison, WI*

MP 010 **High Resolution and High Mass Accuracy Multiply Charged MALDI Technique for in situ Protein Characterization – Sequencing, Identification and Visualization;** [Bingming Chen](#)¹; [Christopher Lietz](#)²; [Anh Van](#)¹; [Lingjun Li](#)^{1,2}; ¹*School of Pharmacy, UW-Madison, Madison, WI*; ²*Department of Chemistry, UW-Madison, Madison, WI*

MP 011 **Optimization of the Analysis of Proteins Found in Paint Cross-sections from Works of Art by MALDI MSI;** [Emily O'Neill](#)¹; [Marcel Powers](#)²; [Julie Arslanoglu](#)³; [John Allison](#)²;

- Richard A. Yost¹; ¹University of Florida, Gainesville, FL; ²The College of New Jersey, Ewing, NJ; ³The Metropolitan Museum of Art, New York, NY
- MP 012 **Development of Imaging MS Methods to Monitor the Molecular Composition of Latent Fingermarks; Nidia Lauzon**¹; Matthew Howland²; Martin Dufresne¹; Vinita Chauhan²; Pierre Chaurand¹; ¹Université de Montréal, Montreal, Canada; ²Health Canada, Ottawa, Canada
- MP 013 **Increasing the Specificity and Sensitivity in Imaging Mass Spectrometry: Regiospecific Transfer of Proteins from Tissue Sections to Functionalized Surfaces; Erik Fournaise**; Pierre Chaurand; Department of Chemistry, Université de Montréal, Montreal, QC, Canada
- MP 014 **Multiplexed Molecular Imaging Mass Spectrometry: Analysis of Different Molecular Types on a Single Tissue Section; Domenico Taverna**^{1,2}; Erin H Seeley^{2,3}; Jeremy L Norris²; Raf Van de Plas²; Giovanni Sindona¹; Richard M Caprioli²; ¹University of Calabria, Arcavacata Di Rende, Italy; ²Vanderbilt University, Nashville, TN; ³Protea Bioscience, Inc., Morgantown, WV
- MP 015 **Top-Down and Bottom-Up Analyses of Proteins on the Same Tissue Section using High Mass Resolution Imaging Mass Spectrometry; David G. Rizzo**; Jeffrey M. Spraggins; Kristie L. Rose; Richard M. Caprioli; Vanderbilt University MSRC, Nashville, TN
- MP 016 **Low Molecular Weight Proteins Revealed by Virtual 2D Gels; Karen Lohnes**; Robert Gunsalus; Joseph A. Loo; Rachel O. Loo; UCLA, Los Angeles, CA
- MP 017 **Single-step Process for Coupling *in situ* Protease Digestion with MALDI IMS: Pre-coated Trypsin Targets for High-throughput Analysis of FFPE Tissues; Faizan Zubair**; Junhai Yang; Richard Caprioli; Paul Laibinis; Vanderbilt University, Nashville, TN
- MP 018 **Tuning the Selectivity of MALDI Imaging Mass Spectrometry through Control of the Sample Preparation Parameters of Alternative Matrix Deposition Techniques; Brian Malys**; Kevin Owens; Elsa Gorre; Drexel University, Philadelphia, PA
- Imaging MS: Software, 019 - 030**
- MP 019 **CARDINAL: Open-source R Package for Statistical Analysis of 2D and 3D Mass Spectrometry Imaging Experiments; Kyle Bemis**¹; Livia Eberlin¹; Christina Ferreira¹; Stephanie van de Ven²; Parag Mallick²; Mark Stolzowicz²; Olga Vitek¹; ¹Purdue University, West Lafayette, IN; ²Stanford School of Medicine, Palo Alto, CA
- MP 020 **Topographical Surface Imaging Mass Spectrometry; Theodore Alexandrov**^{1,2}; Christopher M Rath³; Amina Bouslimani¹; Carla Porto Da Silva¹; Yi Zeng¹; Neha Garg¹; Cliff Kapon¹; Tal Luzzatto Knaan¹; Katherine Duncan⁴; Laura Sanchez¹; Alexey Melnik¹; Kathleen Dorrestein¹; Pieter Dorrestein¹; ¹Skaggs School of Pharmacy, UCSD, La Jolla, CA; ²University of Bremen, Bremen, Germany; ³Novartis Institute for Biomedical Research, Emeryville, CA; ⁴Scripps Institution of Oceanography, UCSD, La Jolla, CA
- MP 021 **3D MALDI Imaging of Mouse Heart after Myocardial Infarction; Michael Becker**¹; Lena Hauberg-Lotte²; Judith Berger³; Janina Oetjen²; Dennis Trede⁹; Michaela Aichler⁶; Wolfgang Dreher⁷; Moritz Wildgruber⁸; Klaus Steinhorst⁵; Jan Hendrik Kobarg⁵; Stefan Schiffler⁹; Stefan Heldmann³; Herbert Thiele³; Peter Maass⁴; Axel Walch⁶; Theodore Alexandrov⁴; ¹Bruker Daltonik GmbH, Bremen, Germany; ²MALDI Imaging Lab, University of Bremen, Bremen, Germany; ³Fraunhofer MEVIS Project Group Image Registration, Lübeck, Germany; ⁴Center for Industrial Mathematics, Bremen, Germany; ⁵Steinbeis Innovation Center SCiLS Research, Bremen, Germany; ⁶Research Unit Analytical Pathology, HMGU München, Oberschleissheim, Germany; ⁷University of Bremen, Bremen, Germany; ⁸Klinikum Rechts der Isar, TU München, München, Germany; ⁹SciLS GmbH, Bremen, Germany
- MP 022 **Automated Differential Analysis Between Tissue Samples Measured by Imaging Mass Spectrometry; Nico Verbeeck**^{1,2}; Yousef El Aalamat^{1,2}; David M. Anderson³; Zsolt Ablonczy⁴; Yiannis Koutalos⁴; Rosalie Crouch⁴; Kevin L. Schey³; Richard M. Caprioli³; Bart De Moor^{1,2}; Etienne Waelkens⁵; Raf Van de Plas³; ¹KU Leuven, ESAT - STADIUS, Leuven, Belgium; ²KU Leuven, iMinds Department Medical IT, Leuven, Belgium; ³Vanderbilt University, MSRC, Nashville, TN; ⁴Medical University of South Carolina, Charleston, SC; ⁵KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium
- MP 023 **Capitalizing on Multi-Modal Imaging: Deeper Insights Through Fusion of Mass Spectrometry and Other Imaging Technologies; Raf Van de Plas**; Junhai Yang; Jeffrey Spraggins; Richard M. Caprioli; Vanderbilt University, Nashville, TN
- MP 024 **OpenMSI: A Web-Based Portal for Rapid Processing of Size-Independent, Next-Generation Mass Spectrometry Imaging Experiments; Ben Bowen**; Annette Greiner; Shreyas Cholia; Katherine Louie; Wes Bethel; Trent Northen; Oliver Ruebel; Lawrence Berkeley National Lab, Berkeley, CA
- MP 025 **Large MSI Datasets Analysis and Normalization using a "BigData" Platform: Proof-of-Concept in Hunting Biomarkers of Pulmonary Arterial Hypertension; Sébastien J. Dumas**¹; Raphael Legouffe²; Fabien Pamelard²; David Bonnel²; Youssef Oulamine²; Gaël Picard De Muller²; Gregory Hamm²; Elie Fadel^{1,3}; Marc Humbert^{1,4}; Sylvia Cohen-kaminsky¹; Jonathan Stauber²; ¹INSERM UMR-S 999, Univ Paris-Sud, LabEx LERMIT, Le Plessis Robinson, France; ²ImaBiotech, MS Imaging Dept., LOOS, France; ³Hôpital Marie Lannelongue, Département de chirurgie, Le Plessis Robinson, France; ⁴Service de Pneumologie, Centre National de Referen, Le Kremlin Bicêtre, France
- MP 026 **Data Management for Handling Large Data Sets in msiQuant Software for Mass Spectrometry Imaging; Patrik Kallback**; Mohammadreza Shariatgorji; Anna Nilsson; Per E. Andren; Uppsala University, Uppsala, Sweden
- MP 027 **Registration of Mass Spectrometry Imaging datasets to the Allen Brain Atlas; Ricardo J. Carreira**¹; Walid M. Abdelmoula²; Reinald Shyti³; Benjamin Balluff¹; René J. M. van Zeijl¹; Else Tolner^{3,4}; Arn M.J.M. van den Maagdenberg^{3,4}; Boudewijn F.P. Lelieveldt^{2,5}; Jouke Dijkstra²; Liam McDonnell¹; ¹Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands; ²Department of Radiology, LUMC, Leiden, Netherlands; ³Department of Human Genetics, LUMC, Leiden, Netherlands; ⁴Department of Neurology, LUMC, Leiden, Netherlands; ⁵Faculty of EEMCS, Delft University of Technology, Delft, Netherlands
- MP 028 **Compositional Hierarchies for Spectral Segmentation of Mass Spectrometry Imaging Data Sets for Redundancy Reduction and Improved Interpretation; Alan M. Race**¹; Josephine Bunch²; Aleš Leonardiš¹; Iain B. Styles¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, London, UK
- MP 029 **Efficient Noise Reduction in Imaging Mass Spectrometry Data using Robust PCA; Yousef El Aalamat**^{1,2}; Nico Verbeeck^{1,2}; Junhai Yang³; Bart De Moor^{1,2}; Richard M. Caprioli³; Etienne Waelkens⁴; Raf Van de Plas³; ¹KU Leuven, ESAT-STADIUS, Leuven, Belgium; ²KU Leuven, iMinds Department Medical IT, Leuven, Belgium; ³Vanderbilt University, MSRC, Nashville, TN; ⁴KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium

MP 030 **Correcting Mass Shifts: Lock Mass-Free Recalibration Procedure for Mass Spectrometry Imaging;** Purva Kulkarni^{1,2}; Philipp Kynast^{1,2}; Filip Kaftan^{2,3}; Vladimír Vrkoslav⁴; Josef Cvačka^{3,4}; Markus Knaden²; Aleš Svatoš^{2,3}; Sebastian Böcker¹; ¹Lehrstuhl für Bioinformatik, FSU, Jena, Germany; ²Max Planck Institute for Chemical Ecology, Jena, Germany; ³Inst. of Organic Chemistry & Biochemistry, AS CR, Prague, Czech Republic; ⁴Dept. of Analytical Chemistry, Charles University, Prague, Czech Republic

Informatics: Workflow & Data Management, 031 - 049

MP 031 **PROCESS – PROteomics Data Collection, Software and Standards to Support Open Access and Long Term Management of Data;** Simon Perkins¹; Henning Hermjakob²; Andrew Jones¹; ¹University of Liverpool, Liverpool, UK; ²European Bioinformatics Institute, Cambridge, UK

MP 032 **Collecting and mining Mass Spectrometry Quality Control Data for Proteomics;** Wout Bittremieux¹; Pieter Kelchtermans²; Dirk Valkenborg³; Lennart Martens²; Bart Goethals¹; Kris Laukens¹; ¹University of Antwerp, Antwerp, Belgium; ²Ghent University, Ghent, Belgium; ³VITO, Mol, Belgium

MP 033 **Community-based Development and Evaluation of Biological Mass Spectrometry Software via the Galaxy Tool Shed;** Bart Gottschalk²; Pratik Jagtap¹; Harald Barsnes³; Marc Vaudel³; Ira Cooke⁴; James Johnson²; John Chilton⁵; Leeann Higgins¹; Todd Markowski¹; Trevor Wennblom²; Anne-Francoise Lamblin²; Yue Chen⁶; Sangtae Kim⁷; Lennart Martens⁸; Tim Griffin⁶; ¹Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN; ²Minnesota Supercomputing Institute, UMN, Minneapolis, MN; ³University of Bergen, Bergen, Norway; ⁴La Trobe University, Melbourne, Australia; ⁵PennState University, University Park, PA; ⁶University of Minnesota, Minneapolis, MN; ⁷Pacific Northwest National Laboratory, Richland, WA; ⁸Ghent University, Ghent, Belgium

MP 034 **KYSS: Mass Spectrometry Data Quality Assessment for Protein Analysis and Large-Scale Proteomics;** Gerard Such-Sanmartin; Simone Sidoli; Estela Ventura-Espejo; Ole Jensen; ^{University of Southern Denmark, Odense, DK}

MP 035 **Modular Software for Visualization, Analysis and Interpretation of Mass-Spectrometry Data;** Dmitry Avtonomov; Chih-Chiang Tsou; Alexander Raskind; Alexey Nesvizhskii; ^{University of Michigan, Ann Arbor, MI}

MP 036 **Using Maxquant on Amazon Cloud EC2: Pros and Cons;** John Philip; Ronald Hendrickson; ^{Memorial Sloan-Kettering Can, New York, NY}

MP 037 **Scientific Workflows for Automated, Documented and Reproducible Data Analysis in Bottom-up and Targeted Proteomics;** Yassene Mohammed^{1,2}; Suzanne van der Plas-Duivesteyn¹; Dominik Domanski³; Christoph Borchers^{2,4}; Magnus Palmblad¹; ¹Center for Proteomics and Metabolomics, Leiden Univ, Leiden, The Netherlands; ²University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ³Instit. of Biochem & Biophys, Polish Acad of Sci, Warsaw, Poland; ⁴UVic Dept of Biochemistry and Biophysics, Victoria, Canada

MP 038 **Bioanalytical Laboratory Data Flow Strategy for Electronic Notebook and Laboratory Information Data Systems;** Michael J. Hayes; Jennifer Davis; Timothy Bedman; Jimmy Flarakos; ^{Novartis Institutes for Biomedical Research, East Hanover, NJ}

MP 039 **Instrument Management and Tracking System Developed for The University of Maryland Baltimore Mass Spectrometry Center;** Michael C. Wilson; Young Ah Goo; Maureen A. Kane; Jace W. Jones; Bao Q. Tran;

Scott Heron; David R. Goodlett; ^{University of Maryland, Baltimore, Baltimore, MD}

MP 040 **Computational Infrastructure for Mining “Big” Proteomic Data;** Himanshu Grover; David Fenyo; ^{New York University, New York, NY}

MP 041 **ProteomicsDB: Show Cases for Rapid Meta-Analysis of Thousands of Mass Spectrometry Data Sets;** Mathias Wilhelm¹; Judith Schlegel²; Hannes Hahne¹; Amin Moghaddas Gholami¹; Marcus Lieberenz²; Emanuel Ziegler²; Lars Butzmann²; Siegfried Gessulat²; Harald Marx¹; Mikhail Savitski³; Karsten Schnatbaum⁴; Ulf Reimer⁴; Holger Wenschuh⁴; Marcus Bantscheff³; Anja Gerstmair²; Franz Faerber²; Bernhard Kuster¹; ¹Technische Universität München, Freising, DE; ²SAP AG Germany, Walldorf, DE; ³Cellzome, Heidelberg, DE; ⁴JPT Peptide Technologies, Berlin, DE

MP 042 **RAId’s Knowledge Integrated Databases;** Gelio Alves; Aleksey Ogurtsov; Yi-Kuo Yu; ^{National Center for Biotechnology Information, NLM, Bethesda, MD}

MP 043 **Enabling Reusable Crowdsourced Annotation of All Mass Spectrometry Data;** Jeremy Carver¹; Mingxun Wang^{1,2}; June Snedecor^{1,2}; Seungjin Na^{1,2}; Adrian Guthals^{1,2}; Nuno Bandeira^{1,2}; ¹Center for Computational Mass Spectrometry, La Jolla, CA; ²University of California, San Diego, La Jolla, CA

MP 044 **Improving Dynamic Offline Lockmass to Tolerate High Mass Shift;** Ying Zhang; Zhihui Wen; Michael Washburn; Laurence Florens; ^{Stowers Institute for Medical Research, Kansas City, MO}

MP 045 **Quality By Design Method Development with Mass Detection;** Sean Mccarthy; Margaret Maziarz; ^{Waters, Milford, MA}

MP 046 **Tracking Chromatographic Peaks with Mass Detection during Method Development;** Margaret Maziarz; Sean Mccarthy; ^{Waters, Milford, MA}

MP 047 **Automated Collision Cross Section Calculation for Traveling Wave Ion Mobility Spectrometry Instruments;** Brett Harper¹; Matthew Brantley²; Michael Pettit¹; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²University of Texas at Tyler, Tyler, TX

MP 048 **A Method for Creating Libraries of Recurring Identified Mass Spectra from Large Metabolic Data Sets;** Wm. Gary Mallard¹; N. Rabe Andriamaharavo¹; Yuri Mirokhin¹; John M. Halket²; Stephen Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²Mass Spectrometry Facility, King’s College, London, UK

MP 049 **Characterizing Molecular Mechanisms of Mammalian Hibernation via Non-Model Organism Quantitative Proteogenomics;** Katie Vermillion¹; Pratik Jagtap²; Todd Markowski²; LeeAnn Higgins²; James Johnson²; Matthew Andrews¹; Timothy Griffin²; ¹University of Minnesota, Duluth, MN; ²University of Minnesota, Minneapolis, MN

Informatics: Small Molecule Identification and Characterization, 050 - 062

MP 050 **Isomer-Specific Fragmentation Pathways of Gaseous Anions Derived from Isomeric Hydroxybenzyl Alcohols (HBAs);** Hanxue Xia; Upul Nishshanka; Carl Weisbecker; Athula B. Attygalle; ^{Stevens Institute of Technology, Hoboken, NJ}

MP 051 **Improved and Extended Tandem Mass Spectral Library with Multiple Precursor Types for More Robust and Flexible Metabolite Identification;** Xiaoyu Yang; Pedatsur Neta; Yuxue Liang; Stephen Stein; ^{National Institute of Standards and Technology, Gaithersburg, MD}

- MP 052 **Large-Scale Analysis of Non-Targeted LC-MS Metabolomics Data with OpenMS in the Compound Discoverer Platform;** [Fabian Aicheler](#)¹; Timo Sachsenberg¹; Erhan Kenar¹; Sebastian Kusch²; Hans Grensemann²; Oliver Kohlbacher¹; ¹Center for Bioinformatics, Tübingen, Germany; ²Thermo Fisher Scientific GmbH, Bremen, Germany
- MP 053 **Application of Fragmentation Analysis in Annotation of Ions in Creation of LC/MS Libraries from Accurate Mass Spectrometry in Global Metabolomics;** [Hongping Dai](#); Corey DeHaven; Anne Evans; *Metabolon, Inc., Durham, NC*
- MP 054 **Combined Isotopic Enrichment, High-Resolution MS, and Advanced Software Tools to Aid in the Identification of Trace-Level Environmental Metabolites by LC/MS;** [Jesse L. Balcer](#)¹; Jeffrey R. Gilbert¹; Yelena A. Adelfinskaya¹; Leah Luna²; Jeffrie Godbey¹; Pete L. Johnson¹; Gerrit J. DeBoer¹; Ayanna U. Jackson¹; Amber R. Mahan¹; ¹Dow AgroSciences, Indianapolis, IN; ²The Dow Chemical Company, Midland, MI
- MP 055 **Web-Based Toolkit for Interpretation of High Accuracy Mass-Spectrometry Data;** Alexander Raskind; *University of Michigan, Ann Arbor, MI*
- MP 056 **Enabling High Throughput Compound Discovery via Global Natural Products Social Molecular Networking;** [Mingxun Wang](#)¹; Yao Peng¹; Jeremy Carver¹; Vanessa Phelan¹; Laura Sanchez¹; Jeramie Watrous¹; Clifford Capono¹; Don Nguyen¹; Tal Knaan¹; Neha Garg¹; Carla Porto Da Silva¹; Amina Bouslimani¹; Alexey Melnik¹; Michael Meehan¹; Wei-ting Liu²; Anne Lamsa¹; Paul Boudreau¹; Evgenia Glukhov¹; Eduardo Esquenazi⁴; Hailey Houson⁴; Venkat Macherla⁴; Mario Sandoval-Calderon⁵; Pep Charusanti¹; Brendan Duggan¹; Marcelino Gutierrez⁶; Xueting Liu³; Lixin Zhang³; Bradley Moore¹; William Gerwick¹; Pieter Dorrestein¹; Nuno Bandeira¹; ¹University of California, San Diego, La Jolla, CA; ²Stanford University, Stanford, CA; ³IMCAS, Beijing, PRC; ⁴Sirenas Marine Discovery, San Diego, CA; ⁵National Autonomous University of Mexico, Mexico City, Mexico; ⁶INDICASAT, Clayton, City of Knowledge, Panama
- MP 057 **Towards Comprehensive, Reliable and Accurate Mass Spectral Data Repositories;** [Eva Duchoslav](#)¹; Lyle Burton¹; Emmanuel Varesio²; Ron Bonner¹; Gérard Hopfgartner²; ¹AB Sciex, Concord, Canada; ²University of Geneva, Geneva, Switzerland
- MP 058 **Spectral Deconvolution of Multiplex Fragmentation Data without the use of a non-Fragmentation Scan;** [Thomas McClure](#); David Wright; Michael Athanas; *Thermo Fisher Scientific, San Jose, CA*
- MP 059 **Machine Classification Consistent with LipidMaps Ontology: Bringing Classifications to the Unknowns;** Ryan Taylor; [Ryan Miller](#); John Prince; *Brigham Young University, Provo, UT*
- MP 060 **Msplinter: A Molecular Model of Lipid Fragmentation;** [Ryan Taylor](#); Ryan Miller; John Prince; *Brigham Young University, Provo, UT*
- MP 061 **XPeak: Quantitation and Characterization of the Metabolic Profile of Colorectal Cancer Relapse;** [Jordan Kruger](#); Amrita Cheema; Subha Madhavan; Nathan Edwards; *Georgetown University Medical Center, Washington, District of Columbia*
- MP 062 **Power of Isotopic Fine Structure for Unambiguous Determination of Metabolite Elemental Compositions: in silico Evaluation and Metabolomic Application;** [Daisuke Miura](#)¹; Tatsuhiko Nagao¹; Daichi Yukihira¹; Yoshinori Fujimura²; Kazunori Saito³; Katsutoshi Takahashi⁴; ¹Kyushu University, Fukuoka, Japan; ²ICMRN, Kyushu University, Fukuoka, Japan; ³Bruker Daltonics K.K., Kanagawa, Japan; ⁴National Institute of Advanced Industrial Science, Tsukuba, Japan
- Proteins: General, 063 - 087**
- MP 063 **Development of an Asp-N Peptide Mapping Method for a Therapeutic Growth Factor;** [Hung-Yu Lin](#); Kenneth Moore; Jenny Heidbrink Thompson; WenJun (David) Mo; *MedImmune, Inc., Gaithersburg, MD*
- MP 064 **Global Effects of Protease Inhibitors on Protein Identification and Quantification;** [John Mangrum](#); Adam Hawkrige; *Virginia Commonwealth University, Richmond, VA*
- MP 065 **Simple Protein Fractionation Enhances Peptide-based Protein Quantitation in Experiments using Metabolic Labeling;** [James Moresco](#)¹; Antonio Pinto²; Jolene Diedrich¹; Patricia Tu¹; John R. Yates III¹; ¹The Scripps Research Institute, La Jolla, CA; ²CAPES Foundation, Brasilia, Brazil
- MP 066 **Effects of Aptamer End Groups on Linkage to Support Material for Specific Enrichment of Proteins;** Funda Yıldırım¹; Ülkü Güler¹; Burak Tavşanlı²; Ömür Çelikbıçak¹; [Bekir Salih](#)¹; ¹Hacettepe University, Department of Chemistry, Ankara, Turkey; ²Istanbul Tech. University, Department of Chemistry, Istanbul, Turkey
- MP 067 **Characterization by nano-LC/ESI-MS/MS of Highly Degraded Collagen Detected in 4,400-year-old Egyptian Wall Paintings of the Idout Tomb;** [Shunsuke Fukakusa](#)¹; Kazuki Kawahara²; Ahmed Sayed Shoeib³; Abel Akarish⁴; Hideya Kawasaki⁵; Hiroshi Suita⁵; Ryuichi Arakawa⁵; Takashi Nakazawa¹; ¹Nara Women's University, Nara, Japan; ²Osaka University, Osaka, Japan; ³Cairo University, Cairo, Egypt; ⁴National Research Center, Cairo, Egypt; ⁵Kansai University, Osaka, Japan
- MP 068 **The Study of Protein/Pigment Interactions in Art Materials from Replica Paints with an Integrated ELISA and Proteomics Approach;** [Natalya Atlasevich](#)¹; Caroline Tokarski³; Brian Baade^{2, 5}; John Loike⁴; Julie Arslanoglu¹; ¹Metropolitan Museum of Art, New York, NY; ²University of Delaware, Newark, DE; ³USR CNRS 3290 MSAP, Villeneuve D'ascq, France; ⁴Columbia University, New York, NY; ⁵University of Delaware, Newark, DE
- MP 069 **Analysis of Centipede, Spider, and Snake Venoms by Electrospray and MALDI Mass Spectrometry;** [Chip Cochran](#); Allen Cooper; Eric Gren; Wayne Kelln; David Nelsen; Ben Gardner; William Hayes; Gerard Fox; *Loma Linda University, Loma Linda, CA*
- MP 070 **High-throughput Scheduled MRM for Multiplexed Analysis of Activity-based Probe Labeled Enzymes in Human Cells;** [Song Li](#); Yu Shi; Christian Malapit; Amy Howell; Xudong Yao; *University of Connecticut, Storrs, CT*
- MP 071 **A Comparative Study of Human Whey Colostral Protein Levels from Women With and Without Gestational Diabetes Mellitus (GDM);** [Darren Weber](#)¹; Jennifer T. Smilowitz^{2, 3}; Dmitry Grapov⁴; Brett S. Phinney¹; ¹Proteomics Core Facility, UC Davis, Davis, CA; ²Foods for Health Institute, UC Davis, Davis, CA; ³Department of Food Science and Technology, UC Davis, Davis, CA; ⁴West Coast Metabolomics Center, UC Davis, Davis, CA
- MP 072 **MS Analyses of Proteins Associated with Autoimmune Diseases;** [Leesa Deterding](#); Jeffrey F. Kuhn; Katina Johnson; Rachelle Bienstock; Jinglan Wang; Erin Hopper; Shyamal Peddada; Frederick Miller; Kenneth B. Tomer; *NIHES, Research Triangle Park, NC*
- MP 073 **Identification of ERK2 Substrates using Label-Free Approach;** Farzin Gharahdaghi; *Astrazeneca, Waltham, MA*

- MP 074 **Evaluation of a Universal LC-MS/MS Assay for Bioanalysis of Human IgG4 Subclass Monoclonal Antibody Protein Drugs;** [Craig Titsch](#); Hao Jiang; Weifeng Xu; Jianing Zeng; Michael Furlong; Mark Arnold; Anne-Francoise Aubry; *Bristol-Myers Squibb, Lawrenceville, NJ*
- MP 075 **Simultaneously Probing Lipoprotein and Lipid Kinetics in Humans using a Practical Oral Tracer Procedure;** [Haihong Zhou](#)¹; Gissette Reyes-Soffer²; Tiffany Thomas²; Kithsiri Heratch¹; Ablatt Mahsut¹; Yi Pan¹; Gowri Bhat¹; Kristian Jensen¹; David Kelley¹; Henry Ginsberg²; Stephen Previs¹; Thomas Roddy¹; ¹*Merck & Co., Inc., Rahway, NJ*; ²*Columbia University, New York, NY*
- MP 076 **Protective Effects of Flavonoids on Cytochrome c Oxidation in Continuous Stirred Tank Reactor Coupled with Electrospray Ionization Mass Spectrometry;** [Hui Fan](#); Veronica Waybright; Jeremy Barnes; Kevin Schug; *The University of Texas at Arlington, Arlington, TX*
- MP 077 **Differential Analysis by SIEVE for sequence Variant Analysis (SVA) of High-Cell-Age Material;** [Georg Drabner](#); Verena Niggeloh; *Roche Diagnostics GmbH, Penzberg, Germany*
- MP 078 **Capillary Electrophoresis Separation and Fractionation Combined with MALDI-MS for Analysis of Reproduction Proteins from Pieridae Butterflies;** Måns Ekelöf; Maria Kihon Rokhas; Johan Jacksén; [Åsa Emmer](#); *Royal Institute of Technology, Stockholm, Sweden*
- MP 079 **Automatic Capillary Isoelectric Focusing – Electrospray Ionization – Mass Spectrometry for Protein Separation and Characterization;** Shuai Sherry Zhao; *University of British Columbia, Vancouver, Canada*
- MP 080 **Capillary Zone Electrophoresis–Electrospray Ionization-Tandem Mass Spectrometry for Top-Down Characterization of the *Mycobacterium marinum* Secretome;** [Yimeng Zhao](#)¹; Liangliang Sun¹; Matthew Champion¹; Michael Knierman²; Norman Dovichi¹; ¹*University of Notre Dame, South Bend, IN*; ²*Eli Lilly and Company, Indianapolis, IN*
- MP 081 **On the Stabilization of Noncovalent Protein Complexes via Vapor Treatment of Electrospray Droplets;** [J. Corinne DeMuth](#); Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- MP 082 **Determination of Novel Copper Binding Sites in MEK1 by Metal-Catalyzed Oxidation Based Mass Spectrometry Analysis;** [Xiaojie Yao](#); Donita Brady; Christopher Counter; Kunhong Xiao; *Duke University Medical Center, Durham, NC*
- MP 083 **Top Down Protein Analysis Applied to Ancient Photographs;** Austin Nevin²; Fabrice Bray¹; Christian Rolando¹; [Caroline Tokarski](#)¹; ¹*Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France*; ²*Politecnico di Milano, Milano, Italy*
- MP 084 **Front-End Electron Transfer Dissociation Coupled to 14.5 T FT-ICR MS for Top-Down Protein MS/MS Analysis;** [Chad R. Weisbrod](#)¹; A. Michelle English²; Nathan K. Kaiser¹; Christopher L. Hendrickson¹; Greg T. Blakney¹; Xiaoyan Guan¹; John E. P. Syka³; Lee Earley³; Christopher Mullen³; Donald F. Hunt²; Alan G. Marshall^{1,4}; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*University of Virginia, Charlottesville, VA*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Florida State University, Tallahassee, FL*
- MP 085 **Semi-preparative Purification and Characterization of Lysozyme Modified with Poly Ethylene Glycol (PEG);** M Sundaram Palaniswamy¹; [N.S Lakshmi](#)¹; Ravindra Gudihall¹; Ning Tang²; ¹*Agilent Technologies, Bangalore, India*; ²*Agilent Technologies, Santa Clara, CA*
- MP 086 **Effect of Centrifugation on Tryptic Digestion;** [Jihyeon Lee](#); Taehee Kim; Jeongkwon Kim; *Chungnam National University, Daejeon, South Korea*
- MP 087 **Systematic and Quantitative Comparison of Digest Efficiency and Specificity Reveals the Impact Of Trypsin Quality on MS-based Proteomics;** Julia Maria Burkhart; [Albert Sickmann](#); *Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
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- MP 088 **Complete Trimethylation of Proteins and its Application to the Quantification of Lysine Methylation at Specific Residues using Mass Spectrometry;** Steven Toth; *Toledo, OH*
- MP 089 **Measuring Protein-Bound Glutathione (PSSG) : Critical Correction for Cytosolic Glutathione Species;** [Michael Bukowski](#); Matthew Picklo; *USDA-ARS Human Nutrition Research Center, Grand Forks, ND*
- MP 090 **Improved Detection of Acidic Post-translational Modifications Utilizing Negative Ion Mode with Alkaline Liquid Chromatography/Fourier Transform-Ion Cyclotron Resonance Mass Spectrometry;** [Phillip McClosky](#); Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- MP 091 **Quantitative Study of Protein Carbonylation in Human Blood Samples;** [Chelsea Coffey](#); Suresh Narayanasamy; David Simpson; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- MP 092 **Methylation Artefacts Introduced during Standard Proteomics Sample Preparation Workflows and Its Impact on Histone PTM Analysis;** [Florian Richter](#)^{1,2}; Aneliya Yoveva¹; Gerhard Mittler¹; ¹*Max Planck Institute of Immunobiology & Epigenetics, Freiburg, Germany*; ²*Functional Proteomics SFB 815 Goethe-University, Frankfurt am Main, Germany*
- MP 093 **Controlled Reduction of Disulfide Bonds in Biopharmaceuticals using an Electrochemical Reactor Cell Online with LC/MS;** [Jean-Pierre Chervet](#); Agnieszka Kraj; Hendrik-Jan Brouwer; Nico Reinhoud; *Antec, Zoeterwoude, Netherlands*
- MP 094 **Characterization of the Degradation Products of a Color-Changed Monoclonal Antibody: Tryptophan-Derived Chromophores;** Yiming Li¹; Alla Polozova²; Flaviu Gruia¹; [Jinhua Feng](#)¹; ¹*MedImmune, Gaithersburg, MD*; ²*Amgen, West Greenwich, RI*
- MP 095 **Linking Epidermal Growth Factor Signaling to Dynamic Chromatin Modifications;** [Rosalynn Molden](#)¹; Daniel Thomas³; Susan Janicki²; Benjamin A. Garcia³; ¹*Princeton University, Princeton, NJ*; ²*The Wistar Institute, Philadelphia, PA*; ³*University of Pennsylvania, Philadelphia, PA*
- MP 096 **Mass Spectrometric Characterization of Aldehyde-Mediated N-terminal Epimerization in Protein;** [Tomoyuki Oe](#); Ryo Kajita; Seon Hwa Lee; Takaaki Goto; *Tohoku University, Sendai, Japan*
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- MP 098 **Modifications of Albumin Isolated from Patients with Multi-Morbid Disease;** [Melissa Grant](#); Iain Chapple; Parth Narendran; Paul Cockwell; Andrew Creese; *University of Birmingham, Birmingham, UK*
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- MP 101 **Global Analysis of Absolute and Relative Quantification of SUMOylated Proteins in *Saccharomyces cerevisiae* by Data-Independent Acquisition using LC/MS^e**; Armann Andaya; Nikhil Bhagwat; Youjin Seo; Neil Hunter; Julie A. Leary; *UC Davis, Davis, CA*
- MP 102 **Quantitative Redox Proteomics using Cysteine Specific Isobaric Tags**; Kumaran Sivagnanam; Leslie M. Hicks; *University of North Carolina, Chapel Hill, NC*
- MP 103 **Analysis of TOR's Role in Lipid Droplet Accumulation in *Chlamydomonas reinhardtii***; Emily Werth¹; Silas P. Rodrigues^{1,2}; Leslie M. Hicks¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, NC*; ²*Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*
- MP 104 **Rapid Profiling of Proteomes and Sub-Proteomes on the Orbitrap Tribrid Mass Spectrometer**; Steven Danielson¹; Todd Markowski²; LeeAnn Higgins²; Pratik Jagtap²; Tim Griffin^{2,3}; Yue Chen³; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN*; ³*Dept. of Biochemistry, University of Minnesota, Minneapolis, MN*
- MP 105 **Comprehensive Screening of lipid Peroxidation-Derived Modifications to Protein using Isotope Data Dependent Scan**; Ryo Takahashi; Seon Hwa Lee; Takaaki Goto; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 106 **Analysis of Glycosylation Sites within the Polypeptide Encoded by Exon 7 of Mouse ZP3 protein (ZP3E7)**; Armand Ngounou; Izabela Sokolowska; Urmi Roy; Alisa Woods; Costel Darie; *Clarkson University, Potsdam, NY*
- MP 107 **Oxidative Stress-Derived Formation and Transamination of N-terminal Alpha-Ketoamide Peptides/Proteins**; Seon Hwa Lee; Hyunsook Kyung; Ryo Yokota; Takaaki Goto; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 108 **Simultaneous Mass Spectrometric Analysis of Various Chemical Modifications on Human Serum Albumin: Strategies for Clean-Up, Sequence Coverage, and Identification**; Takaaki Goto; Yuta Kudo; Kazuyuki Murata; Seon Hwa Lee; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 109 **Unravelling the Drugable ALK Signaling Pathway in Neuroblastoma by Quantitative Proteomics**; Dorte B. Bekker-Jensen; Kristina B. Emdal; Chiara Francavilla; Jesper V. Olsen; *NNF Center for Protein Research, Copenhagen, Denmark*
- MP 110 **Top-down Mass Spectrometry Reveals Molecular Heterogeneity in the Swine Heart**; Zachery Gregorich¹; Wei Guo²; Timothy Hacker¹; Ying Ge¹; ¹*UW Madison, Madison, WI*; ²*University of Wyoming, Laramie, WY*
- MP 111 **Characterization of Cyanobacterial Photosystem II Proteins from Wild-Type and Mutant Cells by Top-Down Mass Spectrometry**; Daniel A. Weisz; Haijun Liu; Weidong Cui; Hao Zhang; Michael L. Gross; Himadri B. Pakrasi; *Washington University in St. Louis, St. Louis, MO*
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- MP 125 **Exploring the Surface Proteins of Myeloid Derived Suppressor Cells**; Sitara Chauhan¹; Steve Danielson²; Rebecca Rose¹; Susan Ostrand-Rosenberg³; Nathan Edwards⁴; Catherine Fenselau¹; ¹*University of Maryland, College Park, MD*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*University of Maryland, Baltimore County, MD*; ⁴*Georgetown University Medical Center, Washington D.C., DC*

- MP 126 **Quantification of Membrane Bound Drug Transporter Proteins at the Blood-Brain Barrier;** Thomas Lau^{1,2}; Jean-Pierre Eliane³; Lauren Gauthier²; Bo Feng³; Patrick Trapa⁴; Jennifer Liras⁴; Hendrik Neubert²; Steven A. Carr¹; ¹Broad Institute, Cambridge, MA; ²Pfizer Inc, Andover, MA; ³Pfizer Inc, Groton, CT; ⁴Pfizer Inc, Cambridge, MA
- MP 127 **Proteomic Analysis of the Membrane Proteins in Human Placenta;** Jong-Sun Lim¹; Hyoung-Joo Lee¹; Keun Na¹; Min Jung Lee¹; Han-Ho Lee¹; Ja-Young Kwon²; Young-Ki Paik¹; ¹YPRC, Seoul, South Korea; ²Collage of Medicine, Yonsei University, Seoul, South Korea
- MP 128 **Characterization of the Membrane Proteome and N-glycoproteome in BV-2 Mouse Microglia by Liquid Chromatography-Tandem Mass Spectrometry;** Dohyun Han^{1,3}; Sungyoon Moon^{1,2}; Jongmin Woo^{1,4}; Youngsoo Kim^{2,3}; ¹Seoul National University College of medicine, Seoul, South Korea; ²Departments of Biomedical Engineering, SNU, Seoul, South Korea; ³Institute of Medical & Biological Engineering, SNU, Seoul, South Korea; ⁴Department of Biomedical Science, Seoul, South Korea
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- MP 135 **A proteomic Approach for Monitoring the Dynamic Response of the Female Oviductal Epithelium Surface to Male Gametes;** Konstantin Artemenko¹; Jana Horáková^{1,4}; Birgit Steinberger^{2,3}; Urban Besenfelder³; Gottfried Brem²; Jonas Bergquist¹; Corina Mayrhofer^{2,3}; ¹Uppsala University, Uppsala, Sweden; ²University of Veterinary Medicine, Vienna, Austria; ³University of Nat.Resources &Applied Life Sciences, Tulln, Austria; ⁴Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
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- MP 137 **Identification and Post-Translational Modifications of Intact Proteins in Exosomes Shed by Murine Myeloid-Derived Suppressor Cells;** Lucia Geis-Asteggiane¹; Avantika Dhabaria¹; Nathan J. Edwards²; Suzanne Ostrand-Rosenberg³; Catherine Fenselau¹; ¹University of Maryland, College Park, MD - Maryland; ²Georgetown University Medical Center, Washington, DC; ³University of Maryland Baltimore County, Baltimore, MD
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- MP 145 **Combining UV Laser Irradiation and IR Activated-Ion Electron Capture Dissociation to Enhance Disulfide Bond Cleavage for Protein Top-Down MS;** Piriya Wongkongkathep¹; Huilin Li¹; Xing Zhang²; Ryan R. Julian²; Rachel O. Loo¹; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA; ²University of California, Riverside, Riverside, CA
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- MP 149 **Top Down Analysis of Protein Classes with Incomplete Genomes;** David Morgenstern¹; Marshall W. Bern²; Chris Becker²; David Fenyó¹; Baldomera Olivera^{3,4}; Julita Imperial³; Beatrix Ueberheide¹; ¹NYU, New York City, NY; ²Protein Metrics Inc., San Carlos, CA; ³University of Utah, Salt Lake City, UT; ⁴The Howard Hughes Medical Institute, Chevy Chase, MD
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- MP 154 **Exploring the Experimental Controls Used for Identifying Transcription Factor Associated Proteins by Mass Spectrometry;** Charles Banks; Zachary Lee; Gina Boanca; Michael Washburn; Stowers Institute, Kansas City, MO
- MP 155 **Intact Mass Analysis of PEGylated Therapeutic Proteins using TripleTOF® System;** Faraz Rashid¹; Annu Uppal¹; Dipankar Malakar¹; Anita Krishnan²; ¹ABSCIEX, Gurgaon, India; ²LUPIN Limited Biotech Division, G O Square Mall, Pune, Maharashtra, IN
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- MP 157 **Increasing Transfer Efficiency in Native Mass Spectrometry of Supermolecular Protein Complexes with a Modified Dual-Funnel QTOF ;** Ralf Hartmer¹; Peter Brechlin¹; Werner Imhoff¹; Anja Wiechmann¹; Wolfgang Jabs¹; Pierre-Olivier Schmitt²; Françoise Debaene³; Alain Van Dorsselaer³; Sarah Cianferani³; ¹Bruker Daltonik, Bremen, Germany; ²Bruker Daltonique, Wissembourg, France; ³LSMBO Université de Strasbourg, Strasbourg, France
- MP 158 **A Proteomic Profile of Deleted in Breast Cancer 1 (DBC1) and its Role in Transcriptional Regulation;** Preeti Joshi; Amanda Guise; Olivia Quach; Sophie Giguere; Jeffrey Kong; Ileana M. Cristea; Princeton University, Princeton, NJ
- MP 159 **Interactome of Bacillus subtilis Cell Division Machinery;** Livia Goto Silva¹; Jimmy Rodriguez Murillo¹; Micaella P. da Fonseca²; Agnelo Rodrigues de Souza²; Gilberto Barbosa Domont¹; Federico Gueiros-Filho³; Magno Junqueira¹; ¹Federal University of Rio de Janeiro, Rio De Janeiro, Brazil; ²University of Brasilia, Brasilia, DF-Brazil; ³University of Sao Paulo-USP, Sao Paulo, Sao Paulo-Brazil
- MP 160 **A Robust Platform for Routine Analysis of Endogenous Protein Complexes with Ion Exchange Chromatography Coupled to Native Electrospray Mass Spectrometry;** Paul Dominic B. Olinares; Zachary T. Quinkert; Julio C. Padovan; Brian T. Chait; The Rockefeller University, New York, NY
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- MP 162 **Comparative proteomic Analysis Reveals Novel Components at the Plasma Membrane of Differentiated HepaRG Cells;** Catalina Petreanu²; Izabela Sokolowska¹; Alina Macovei²; Alisa G. Woods¹; Lucian G Radu²; Costel Darie¹; Norica Brinza-Nichita²; ¹Clarkson University, Potsdam, NY; ²Institute of Biochemistry, Bucharest, Romania
- MP 163 **Defining Interacting Proteins of the Retinoic Acid Receptor Responder Protein-1 using TAP-TAG Affinity and SILAC Titration Strategy;** Haeri Seol; Kristy J Brown; Yetrib Hathout; Children's National Medical Center, Washington, DC
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- MP 165 **Accurate Stoichiometry Determination of a Very Large Molecular Machine: The 50 MDa Yeast Nuclear Pore Complex;** Wenzhu Zhang; Javier Fernandez-Martinez; Michael P. Rout; Brian T. Chait; The Rockefeller University, New York, NY
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- MP 167 **Rapid Gas-Phase Carbene Labeling and Top-Down Mass Spectrometry Provides Topographical Structural Information;** Daniel Therrien²; Douglas Steiner²; Elizabeth Campbell¹; Mark Carver¹; Emily Hammer¹; Margaret Cothorn¹; Paul Martino¹; ¹Carson-Newman University, Jefferson City, TN; ²Martino Labs, Inc., Kalispell, MT
- MP 168 **Chemo-Enzymatic Derivatization and Enrichment of Protein Post-Translational Modifications: Methylation and Isoaspartic Acid;** Zhaohui Zhou; Northeastern University, Boston, MA
- MP 169 **Structural Analysis of Fibrillar and Prefibrillar Oligomeric Forms of Amyloid Abeta at the Level of Single Residue by Covalent Labeling;** Janna Kiselar¹; Alexandra Klinger²; Sergei Ilchenko¹; Mark R Chance¹; Paul Axelsen²; ¹Case Western Reserve Univ, Cleveland, OH; ²University of Pennsylvania, Pennsylvania, PA

- MP 170 **Identification of Phosphorylation of Tyrosines on Tubulin Following Exposure to Organophosphorus Pesticides using LC-MS/MS;** [Michael G. Bartlett](#)¹; [Pei Li](#)¹; [Alvin Terry](#)²; ¹University of Georgia, Athens, GA; ²Georgia Regents University, Augusta, GA
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- MP 240 **Lipidomic Analysis and Comparison of Young and Old Rat Skeletal Muscles using UHPLC-HRMS**; Yu-Hsuan Tsai^{1,2}; Timothy Garrett^{1,3}; Christy Carter^{1,4}; Richard A. Yost^{1,2}; ¹University of Florida, Gainesville, FL; ²Dept. of Chemistry, Gainesville, Florida; ³Dept. of Pathology, Gainesville, Florida; ⁴Dept. Aging & Geriatric Research, Gainesville, Florida
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- MP 248 **Gas Phase Discrimination of Phosphatidylcholines and Phosphatidylethanolamines using Charge-Inversion Ion/Ion Reactions**; Stella Rojas-Betancourt¹; John Stutzman¹; Stephen J Blanksby²; Scott McLuckey¹; ¹Purdue University, West Lafayette, IN; ²Queensland University of Technology, Brisbane, Australia
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- MP 250 **Global Lipid Profiling of Mucosa from Patients with Chronic Sinusitis and Otitis Media and Controls**; Farbod Fazlollahi¹; Kessiri Kongmanas²; Nongnui Tanphaichitr²; Kym Faull¹; Jeffrey Suh¹; Quinton Gopen¹; ¹UCLA, Los Angeles, CA; ²University of Ottawa, Ottawa, Canada
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- MP 252 **Phospholipid Oxidation Products as Biomarkers for Oxidative Stress in Inflammatory Liver Disease**; Beate Fuchs; Jürgen Schiller; University of Leipzig, Leipzig, Germany
- MP 253 **The Use of Glycerol for Enhanced Lipid Signal in Liquid Extraction Surface Analysis Mass Spectrometry of Thin Tissue Sections**; Alexander Dexter¹; Josephine Bunch²; Iain B. Styles¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, London, UK
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- MP 254 **Confetti: A Multi-protease Map of the HeLa Proteome for Comprehensive Proteomics**; Hamid Mirzaei¹; David Trudgian¹; Xiaofeng Guo²; Andrew Lemoff¹; Sivaramakrishna Yadavalli¹; ¹UT Southwestern, Dallas, TX; ²University of Pennsylvania, Philadelphia, PA
- MP 255 **A Draft Map of the Human Proteome**; Min-Sik Kim¹; Sneha M. Pinto^{1,2}; Derese Getnet¹; Raja Sekhar Nirujogi^{1,2}; Srikanth S. Manda^{1,2}; Raghothama Chaerkady¹; Anil Madugundu²; Dhanashree S. Kelkar²; Ruth Isserlin³; Shobhit Jain³; Joji K. Thomas²; Babylakshmi Muthusamy²; Nandini A. Sahasrabudhe²; Praveen Kumar²; Pamela Leal Rojas¹; Lavanya Balakrishnan²; Jayshree Advani²; Bijesh George²; Santosh Renuse²; Lakshmi Dhevi N. Selvan²; Arun H. Patil²; Vishalakshi Nanjappa²; Aneesh Radhakrishnan²; Tejaswini Subbannayya²; Rajesh Raju²; Manish Kumar²; Sreelakshmi Sreenivasamurthy²; Arivusudar Marimuthu²; Gajanan J. Sathe²; Sandip Chavan²; Keshava K. Datta²; Yashwanth Subbannayya²; Apeksha Sahu²; Soujanya D. Yelamanchi²; Savita Jayaram²; Pavithra Rajagopalan²; Jyoti Sharma²; Krishna R. Murthy²; Aafaque A. Khan²; Sartaj Ahmed²; Nazia Syed²; Gourav Dey²; Aditi Chatterjee²; Tai-Chung Huang¹; Jun Zhong⁴; Xinyan Wu¹; Patrick G. Shaw⁴; Muhammad S. Zahari¹; Henry Lam⁵; Christopher J. Mitchell¹; John T. Schroeder¹; Ravi Sirdeshmukh²; Anirban Maitra¹; Steven D. Leach¹; Charles G. Drake¹; Marc K. Halushka¹; T. S. Keshava Prasad²; Ralph H. Hruban¹; Candace L. Kerr⁶; Gary D. Bader³; Christine A. Iacobuzio-Donahue¹; Harsha Gowda²; Akhilesh Pandey¹; ¹Johns Hopkins University SOM, Baltimore, MD; ²Institute of Bioinformatics, Bangalore, India; ³The Donnelly Centre, University of Toronto, Toronto, Canada; ⁴Johns Hopkins University, Baltimore, MD; ⁵The Hong Kong University of Science and Technology, Clear Water Bay, Hongkong; ⁶University of Maryland, Baltimore, Maryland
- MP 256 **Integrative Omics Analysis Reveals Distinct Gene and Protein Expression Signatures across Multiple Tissues in an Individual**; Srikanth S. Manda^{1,3}; Min-Sik Kim²; Raja Sekhar Nirujogi^{1,3}; Premendu P. Mathur³; Harsha Gowda¹; Akhilesh Pandey^{1,2}; ¹Institute of Bioinformatics, Bangalore, India; ²Johns Hopkins University SOM, Baltimore, MD; ³Center for Bioinformatics, Pondicherry University, Puducherry, India
- MP 257 **High-Coverage High-Throughput Characterization of Breast Cancer Cell Lines through the Use of Synchronous Precursor Selection MS3-based 10-plexed Quantitative Proteomics**; John Lapek¹; Jessica Biosvert¹; Cyril Benes^{1,2}; Wilhelm Haas^{1,2}; ¹MGH Cancer Center, Charlestown, MA; ²Harvard Medical School, Charlestown, MA
- MP 258 **Construction of a Physical Map of a Human Cell**; Anne-Claude Gingras¹; Christopher Go¹; Wade H Dunham¹; James DR Knight¹; Étienne Coyaud²; Geoffrey Hesketh¹; Jean-Philippe Lambert¹; Payman Samavarchi-Tehrani¹; Amber L. Couzens¹; Andy Kong³; Laurence Pelletier¹; Hyungwon Choi⁴; Alexey Nesvizhskii³; Brian Raught²

- ¹Lunenfeld-Tanenbaum Research Institute, Toronto, Canada; ²Ontario Cancer Institute, Toronto, Canada; ³University of Michigan, Ann Arbor, MI; ⁴National University of Singapore, Singapore
- MP 259 **The Nuclear Proteome of a Vertebrate; Martin Wuehr**; Thomas Guettler; Leonid Peshkin; Graeme C. McAlister; Aaron C. Groen; Timothy J. Mitchison; Marc W. Kirschner; Steven P. Gygi; *Harvard Medical School, Boston, MA*
- MP 260 **Protein Quantitative Trait Locus (pQTL) Analysis in a Mouse Genetic Reference Population using Targeted Mass Spectrometry Methods; Yibo Wu**¹; Evan Williams²; Sander Houten³; Carmen Argmann³; Witold Wolski¹; Johan Auwerx²; Ruedi Aebersold^{1,4}; ¹IMSB, Zurich, Switzerland; ²EPFL, Lausanne, Switzerland; ³University of Amsterdam, Amsterdam, Netherland; ⁴University of Zurich, Zurich, Switzerland
- MP 261 **A Systems Approach to the Characterization of Toll-Like Receptor Response to Different Ligand Stimulation in Macrophages; Virginie Sjoelund**; Arthur Nuccio; Zachary Benet; Jessica Mann; Marijke Koppenol-Raab; Alisa Bochnowski; Nathan Manes; Bhaskar Dutta; Iain Fraser; Aleksandra Nita-Lazar; *NIH/NIAID/LSB, Bethesda, MD*
- MP 262 **Dynamic Analysis of Pure HIV-1 Infected and Bystander Monocyte Derived Macrophages (MDMs); Isabel Martinez Ferrando**¹; Alexandre Deshiere²; Alexey Lyashkov¹; Ceereena Mohien¹; David Colquhoun¹; Michel Ouellet²; Michel Tremblay²; David R. Graham¹; ¹Johns Hopkins School of Medicine, Baltimore, MD; ²Laval University, Quebec city, Quebec
- MP 263 **Advanced Ti4+-IMAC (Phospho)proteomics to Identify Novel Melanoma Companion Drug Targets and Uncover Phosphorylation Dynamics and Pathway Dependence in Senescence Signaling; Erik L. de Graaf**¹; Gianluca Maddalo¹; Joanna Kaplon²; Marjon A. Smit²; Daniel S. Peeper²; Albert J.R. Heck¹; A.F. Maarten Altelaar¹; ¹Utrecht University, Utrecht, The Netherlands; ²The Netherlands Cancer Institute, Amsterdam, The Netherlands
- MP 264 **Enhanced Informatics Methods for Enriching Protein Identifications in the Metaproteome Characterization of the Human Gut Microbiome; Robert Hettich**¹; Alison Erickson¹; J Chai¹; Chongle Pan²; Rachel Adams¹; Brandi Cantarel³; Claire Fraser-Liggett³; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²Oak Ridge National Lab, Oak Ridge, TN; ³University of Maryland, Baltimore, MD
- MP 265 **A Data Independent Strategy for a Multi-omic Approach to Investigate Obesity Treatment within a Mouse Model; Gertjan Kramer**¹; Nicholas Dekker¹; Lee A Gethings²; Victoria Lee³; Robert J Beynon³; James I Langridge²; Johannes P.C. Vissers²; Johannes M.F.G. Aerts¹; ¹Academic Medical Centre, University of Amsterdam, Amsterdam, Netherlands; ²Waters, Manchester, UK; ³University of Liverpool, Liverpool, UK
- MP 266 **Hypothesis Driven Approach to Integrated Lipidomic and Proteomic Data Analysis; Gogce Crynen**^{1,2}; Laila Abdullah^{1,2}; Jon Reed^{1,2}; James Evans¹; Hannah Montague¹; Ariel Hart¹; Ariel Gonzalez¹; Madison Crocker¹; Tanja Emmerich¹; Robert Pelot¹; Michael Mullan¹; Fiona Crawford^{1,2}; ¹Roskamp Institute, Sarasota, Florida; ²SRQ Bio, Sarasota, Florida
- MP 267 **Comprehensive Analysis of Alterations in Lipid and Bile Acid Metabolism by Carbon Tetrachloride using Integrated Transcriptomics and Metabolomic; Jinchun Sun**¹; Thomas Schmitt¹; Laura Schnackenberg¹; Lisa Pence¹; Yosuke Ando^{1,2}; James Greenhaw¹; Xi Yang¹; Svetoslav Slavov¹; William Salminen^{1,3}; Donna Mendrick¹; Richard Beger¹; ¹NCTR / USFDA, Jefferson, AR; ²Daiichi Sankyo Co., Ltd, Tokyo, Japan; ³PAREXEL International, Boston, MA
- MP 268 **LC-MS Chemoplexing for the Direct Measurement of Apparent Catalytic Efficiency of Enzyme Systems; Richard King**¹; Bonnie Baker¹; Victoria King²; Carmen Fernandez-Metzler¹; ¹PharmaCadence Analytical Services, LLC, Hatfield, PA; ²Northeastern University, Boston, MA
- MP 269 **Chemokine and Sphingosine-1-Phosphate Signaling in RAW 264.7 Cells Quantitated using Targeted Proteomics and Simulated using Simmune; Nathan Manes**¹; Marijke Koppenol-Raab¹; Eunkyung An¹; Virginie Sjoelund¹; Jing Sun¹; Bastian Angermann¹; Masaru Ishii²; Martin Meier-Schellersheim¹; Ronald Germain¹; Aleksandra Nita-Lazar¹; ¹National Institutes of Health, Bethesda, MD; ²Osaka University, Osaka, Japan
- MP 270 **Integrated Transcriptomic and Proteomic Analysis of an Indian Malaria Vector –Anopheles stephensi; Sreelakshmi Sreenivasamurthy**^{1,2}; Ajeet Kumar Mohanty³; Manish Kumar^{1,2}; Gourav Dey^{1,2}; Sneha Pinto^{1,4}; Raja Sekhar Nirujogi^{1,4}; Anil Madugundu¹; Arun Patil¹; Jayshree Advani¹; Sutopa Dwivedi¹; Manoj Kumar Gupta^{1,2}; Dhanashree Kelkar¹; Chris Mitchell⁴; Charles Wang⁵; Harsha Gowda¹; T. S. Keshava Prasad¹; Zhijian Tu⁶; Ashwani Kumar³; Akhilesh Pandey⁴; ¹Institute of Bioinformatics, Bangalore, India; ²Manipal University, Manipal, India; ³National Institute of Malaria Research, Goa, India; ⁴Johns Hopkins University School of Medicine, Baltimore, MD; ⁵School of Medicine, Loma Linda University, Loma Linda, CA; ⁶Department of Biochemistry, Virginia Tech, Blacksburg, VA
- MP 271 **Dysregulation of Nitric Oxide Metabolism in Host Erythrocytes Following Plasmodium falciparum Infection; Simon A. Cobbold**¹; David H. Perlman²; Manuel Llinás³; Kiaran Kirk⁴; ¹Bio21 Institute, University of Melbourne, Melbourne, Australia; ²Princeton University, Princeton, NJ; ³The Pennsylvania State University, University Park, PA; ⁴The Australian National University, Acton, Australia
- MP 272 **Absolute Quantification of Over 1000 Yeast Proteins Provides Insights into Translational Control; Stephen W. Holman**¹; Craig Lawless²; Philip Brownridge¹; Karin Lanthaler²; Victoria M. Harman¹; Dean E. Hammond¹; Rebecca L. Miller¹; Rachel H. Watkins²; Paul F. G. Sims²; Christopher M. Grant²; Claire E. Evers¹; Robert J. Beynon¹; Simon J. Hubbard²; ¹The University of Liverpool, Liverpool, UK; ²The University of Manchester, Manchester, UK
- MP 273 **Proteomic Analysis of Environmental Stress in Oysters; Paul Haynes**¹; Emma Thompson²; Sridevi Muralidharan¹; Wayne O'Connor³; David Raftos²; ¹Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, NSW Australia; ²Department of Biological Sciences, Macquarie University, NSW Australia; ³NSW Department of Primary Industries, Taylors Beach, NSW Australia
- MP 274 **An Integrated Metabolomics and Proteomics Approach to Understand Chemically Mediated Diatom Competition; Christina M. Jones**¹; Kelsey L. Poulson-Ellestad¹; Brook L. Nunn²; Jessie Roy¹; Facundo M. Fernández¹; Julia Kubanek¹; ¹Georgia Institute of Technology, Atlanta, GA; ²University of Washington, Seattle, WA
- MP 275 **Multiple Nutrient Stresses at Intersecting Pacific Ocean Biomes Detected by Protein Biomarkers; Mak Saito**¹; Matthew McIlvin¹; Dawn Moran¹; Tyler Goepfert¹; Giacomo DiTillio²; Carl Lamborg¹; ¹Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; ²College of Charleston, Charleston, SC
- MP 276 **Integrated Omics Analysis of the Interaction Between Ignicoccus hospitalis and Nanoarchaeum equitans; Timothy Hamerly**¹; Brian P. Tripet¹; Richard Giannone²; Robert Hettich²; Mircea Podar²; Valerie Copie¹; Brian

- Bothner¹; ¹Montana State University, Bozeman, MT; ²Oak Ridge National Laboratory, Oak Ridge, TN
- MP 277 **Characterization of the Core and Unique Proteome of *Anaeromyxobacter dehalogenans* 2CP-C Grown With Various Electron Acceptors;** Xiaoxin Liu^{1,2}; Silke Nissen^{1,2}; Karuna Chourey¹; Frank Löffler^{1,2}; Robert Hettich^{1,2}; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²The University of Tennessee, Knoxville, TN
- MP 278 **Targeted Proteogenomic Characterization of the *Shewanella oneidensis* MR-1 Extracellular Proteome;** William Judson Hervey IV¹; Erinn C. Howard²; Emily R. Peterson³; Dagmar Hajkova Leary¹; Anthony P. Malanoski¹; Jinny L. Liu¹; Justin C. Biffinger¹; Sarah M. Glaven¹; Baochuan Lin¹; Lisa A. Fitzgerald¹; Gary J. Vora¹; Bradley R. Ringeisen¹; ¹Naval Research Laboratory, Washington, DC; ²West Virginia Wesleyan College, Buckhannon, WV; ³Nova Research, Inc., Alexandria, VA
- MP 279 **Metaproteomic Analysis of an Electricity Consuming Biocathode Biofilm;** Dagmar Hajkova Leary¹; Anthony Malanoski¹; William Judson Hervey, IV.¹; Zheng Wang¹; Brian Eddie²; Gary Vora¹; Leonard Tender¹; Baochuan Lin¹; Sarah Glaven¹; ¹Naval Research Laboratory, Washington, DC; ²National Research Council, Washington, DC
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- MP 281 **Analysis of Pain Panel Medications in Urine on Raptor™ Biphenyl by LC-MS/MS;** Sharon Lupo; Frances Carroll; Paul Connolly; Ty Kahler; Restek, Bellefonte, PA
- MP 282 **Comparison of LDTD with Traditional LCMS for Quantitative Screening of Urine Drugs of Abuse using Benchtop Quadrupole Orbitrap Mass Spectrometer;** Kristine Van Natta; Marta Kozak; Thermo Fisher Scientific, San Jose, CA
- MP 283 **Evaluation of Sample Preparation Methods for Semi-Quantitative Ultra-High Throughput Urine Screening using LDTD HR/AM MS technique;** Marta Kozak; Kristine Van Natta; Thermo Fisher Scientific, San Jose, CA
- MP 284 **Ultra Fast Analysis of 13 Benzodiazepines by LDTD-MS/MS Cross Validated with LC-MS/MS for 200 Real Urine Samples;** Alex Birsan; Serge Auger; Annick Dion; Pierre Picard; Jean Lacoursiere; Phytrolix Technologies Inc., Quebec, QC
- MP 285 **Evaluation of a Novel High-Throughput Screening Method for Drugs of Abuse in Urine with Paper-Spray Triple Quadrupole Mass Spectrometry;** Bradley Hart¹; Maria C. Prieto Conaway¹; Kristine van Natta¹; Nicholas E. Manicke²; Marta Kozak¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Dept of Chemistry, Indiana Univ-Purdue Univ, Indianapolis, IN
- MP 286 **Rapid LC-MS/MS Analysis of Opiates and Benzodiazepines in Urine using a Partially Porous C-18 Stationary Phase;** J. Fred Banks; Ammon Analytical Laboratory, Linden, NJ
- MP 287 **Challenges and Solutions for High Throughput TFC-LC-MS/MS in Clinical Toxicology;** Yvonne Wright; Christopher Shuford; Matthew Crawford; Patricia Holland; Stacy Dee; Martin Green; Russell Grant; LabCorp, Burlington, NC
- MP 288 **Development of a New Toxicological Drug Screening Method for More than 800 Compounds in Biological Matrices using a UPLC-QToF MS;** Gilles Provencher; Nicolas Caron; Michel Lefebvre; Normand Fleury; INSPQ, Quebec, Canada
- MP 289 **Applying Enhanced Confirmation Criteria for Reducing False Positive Rates (FPR) in Toxicology Screening using High Resolution, LC-QToF, Accurate Mass Analysis;** Petra Decker¹; Karin Wendt¹; Carsten Baessmann¹; Christian Albers¹; Tony Drury²; Laura Huppertz³; Juergen Kempf³; Volker Auwaerter³; Anna Pelander⁴; Mira Sundström⁴; Ilkka Ojanperä⁴; Bruker Daltonik GmbH, Bremen, Germany; ²Bruker UK Ltd., Coventry, UK; ³University Medical Center, Forensic Toxicology, Freiburg, Germany; ⁴Hjelt-Institute, University of Helsinki, Helsinki, Finland
- MP 290 **Quantitation of Pain Management Drugs using Ultra-Fast Liquid Chromatography/Mass Spectrometry in Human Plasma Utilizing Positive/Negative Polarity Switching;** Steven R. McGown¹; Robert D. English¹; Chris Denicola²; Nataliya Bulayeva³; Rob Freeman²; Kevin Rosenblatt³; Ben Figard¹; Shimadzu Scientific Instruments, Houston, TX; ²Restek Corporation, Bellefonte, PA; ³UT-Health Science Center, Houston, TX
- MP 291 **Increased Throughput for the Analysis of delta-9-THC in Oral Fluids using Triple Quadrupole Mass Spectrometry coupled to Automated Dual-Channel HPLC;** Kevin McCann; Andre Szczesniewski; Agilent Technologies, Santa Clara, CA
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- MP 293 **A Workflow-driven High-throughput Screening Method for Synthetic Cannabinoids and Metabolites in Urine with Q-TOF Mass Spectrometer and Multiplexed LCs;** Xiang He; Zhaoxiang (Sean) Wu; Jenny Moshin; Alexandre Wang; AB SCIEX, Redwood City, CA
- MP 294 **Quantification of Illicit Drugs in Urine for Confirmatory Analysis in Routine Laboratories using Ion Trap LC-MSⁿ;** Julian Philips; Markus Peer; Birgit Schneider; Bruker Daltonik, Bremen, Germany
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- MP 296 **Ionization Mechanism in Radio-Frequency Ionization (RFI);** Abayomi D. Olaitan; Behrooz Zekavat; Touradj Solouki; Baylor University, Waco, TX
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- MP 299 **Ionization of Gaseous Compounds in Direct and Dopant-Assisted Atmospheric Pressure Photoionization;** Tiina J Kauppila¹; Hendrik Kersten²; Thorsten Benter²; ¹University of Helsinki, Helsinki, N/A; ²University of Wuppertal, Wuppertal, Germany
- MP 300 **Mechanistic Understanding on Why a Number of Compounds with High Gas Phase Basicity Produce Mostly Molecular Ions by (+) APPI-MS;** Arif Ahmed¹; Cheol Ho Choi^{1,2}; Younghwan Kim³; Sunghwan Kim^{1,2}; ¹Kyungpook National University, Daegu, South Korea; ²Green-Nano Materials Research Center, Daegu, South Korea; ³Korea Basic Science Institute, Daejeon, South Korea

- MP 301 **Ionization from Freezing Water: Why it Should be Expected;** Charles N. McEwen²; Beixi Wang¹; Vincent Pagnotti²; Shubhashis Chakrabarty²; Sarah Trimpin¹; ¹Wayne State University, Detroit, MI; ²University of the Sciences, Philadelphia, PA
- MP 302 **Experimental and Theoretical Investigations of Positron Ionization Mass Spectrometry with Biological Molecules;** Panagiotis Papoulias¹; Indika Wanniarachchi¹; Caroline Morgan¹; Alan Sebastian¹; Larry Burggraf²; Rod Greaves³; ¹Wayne State University, Detroit, MI; ²Air Force Institute of Technology, Dayton, OH; ³First Point Scientific, Inc., Agoura Hills, CA
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- MP 304 **Large Biomolecule Clusters Detection using MALDI Ion Trap Mass Spectrometer with Charge Detector;** Yung-Kun Chuang; Szu-Hsueh Lai; Jung-Lee Lin; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- MP 305 **Ion-to-Neutral Ratios and Thermal Proton Transfer Reactions in Matrix-Assisted Laser Desorption/Ionization;** I-Chung Lu¹; Kuan Yu Chu^{1,2}; Chih-Yuan Lin¹; Yuri A. Dyakov¹; Hsu Chen Hsu¹; Yuan-Tseh Lee^{1,2}; Chi-Kung Ni^{1,3}; ¹Academia Sinica, Taipei, Taiwan; ²National Taiwan University, Taipei, Taiwan; ³National Tsinghua University, Hsinchu, Taiwan
- MP 306 **Ion Intensity and Thermal Proton Transfer Reactions in Matrix-Assisted Laser Desorption/Ionization;** Chuping Lee^{1,3}; I-Chung Lu¹; Hui-Yuan Chen¹; Hou-Yu Lin^{1,3}; Sheng-Wei Hung¹; Yuri Dyakov¹; Kuo-Tung Hsu²; Chih-Yu Liao²; Yin-Yu Lee²; Cheng-Ming Tseng⁵; Yuan Tseh Lee^{1,3}; Chi-Kung Ni^{1,4}; ¹Academia Sinica, Taipei, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ³National Taiwan University, Taipei, Taiwan; ⁴National Tsing Hua University, Hsinchu, Taiwan; ⁵National Chiao Tung University, Hsinchu, Taiwan
- MP 307 **Excited State Lifetime and Fluorescence Properties of UV-MALDI Matrices;** Hou-Yu Lin¹; Botao Song¹; I-Chung Lu¹; Kuo-Tung Hsu²; Chih-Yu Liao²; Yin-Yu Lee²; Cheng-Ming Tseng³; Yuan-Tseh Lee^{1,4}; Chi-Kung Ni^{1,5}; ¹Institute of Atomic and Molecular Sciences, Academ, Taipei, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ³National Chiao Tung University, Hsinchu, Taiwan; ⁴National Taiwan University, Taipei, Taiwan; ⁵National Tsing Hua University, Hsinchu, Taiwan
- MP 308 **Relation of Excited State Lifetimes and Ion Yields for Common MALDI Matrices;** Kristopher Kirmess; Gary R. Kinsel; *Southern Illinois University at Carbondale, Carbondale, Illinois*
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- MP 310 **One Method Might Not be Enough – Investigating Ionization of Peptides and Their Modifications;** Wiebke Nadler^{1,3}; Dietmar Waidelich⁴; Alexander Kerner^{1,3}; Christoph Roesli^{1,2}; ¹Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany; ²Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany; ³Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany; ⁴AB SCIEX, Darmstadt, Germany
- MP 311 **In-Source Reactions of Catechol During Oxidative Positive Ion Electrospray Mass Spectrometric Analysis;** Luis Sojo; *Xenon Pharmaceutical, Burnaby, Canada*
- MP 312 **Protonation and Desolvation as Limiting Factors in the Linear Dynamic Range of Electrospray Ionization Mass Spectrometry;** Clint M. Alfaro; Agbo-Oma Uwakweh; Daniel A. Todd; Brandie M. Ehrmann; Nadja B. Cech; *University of North Carolina at Greensboro, Greensboro, NC*
- MP 313 **Predicting Concentrations of Small Molecules without Standard Substances in LC/API/MS via Ionization Efficiency Scales;** Anneli Kruve; Jaanus Liigand; Piia Burk; Karl Kaupmees; Riin Rebane; Ivo Leito; Koit Herodes; Merit Oss; *University of Tartu, Tartu, Estonia*
- MP 314 **Supercharging Reagents as Mobile Phase Additives in the LC-MS Analysis of Intact Proteins;** Michael Nshanian¹; Rachel R. Ogorzalek Loo²; Joseph A. Loo¹; ¹UCLA, Department of Chemistry and Biochemistry, Los Angeles, CA; ²UCLA, Department of Biological Chemistry, Los Angeles, CA
- MP 315 **Atmospheric Pressure Laser Ionization with a Novel Highly Sensitive Atmospheric Pressure Ionization Interface for Gas Chromatography-Mass Spectrometry;** Thorsten Benter¹; Tiina J Kauppila²; Hendrik Kersten¹; ¹University of Wuppertal, Wuppertal, Germany; ²University of Helsinki, Helsinki, N/A
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- MP 329 **Probing Gold-Catalyzed Alkyne Hydration Reaction by Mass Spectrometry: Evidence for Dinuclear Gold Intermediates and Dual Activation of Substrates;** Mei Lu¹; Yijin Su²; Xiaodong Shi²; Eric Masson¹; Fengyao Li¹; Hao Chen¹; ¹Ohio University, Athens, OH; ²West Virginia University, Morgantown, WV
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- MP 330 **Thermal Ionization Time-of-Flight Mass Spectrometry as a Tool for Uranium Exploration;** Dongfa Guo¹; Shengkai Xie¹; Jinying Li²; Jing Tan¹; Zengwei Fan¹; Guifang Liu¹; Chen Dong¹; Jianyong Cui¹; ¹Beijing Research Institute of Uranium Geology, Beijing, China; ²China Institute of Atomic Energy, Beijing, China
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- MP 433 **A Novel Platform for Plasma Biomarker Discovery with super-SILAC Quantification of Microparticle Proteomes**; Michal Harel¹; Yuval Shaked²; Tamar Geiger¹; ¹Tel Aviv University, Tel Aviv, Israel; ²Technion, Haifa, Israel
- MP 434 **Novel Orbitrap-Based Two-Dimensional LC-MS/MS Workflows to Qualitatively and Quantitatively Analyze Native Human Peptides in Complex Secretome Samples**; Baozhen Shan²; Martijn Pinkse¹; Bharath Kumar Raghuraman¹; Cassandra Wigmore²; Peter D. Verhaert¹; ¹Delft University of Technology, Delft, Netherlands; ²BSI, Waterloo, Ontario, Canada
- MP 435 **Biomarker Discovery of CD14, a Soluble Endotoxin Receptor for Diagnosis of Stable Coronary Artery Disease**; Thomas S.-H. Chiou¹; Min-Yi Lee¹; Chao-Jen Kuo¹; Wen-Jen Chen¹; Chun-Hao Huang¹; Chen-Lung Steve Lin¹; Wen-Ter Lai²; ¹Kaohsiung Medical University, Kaohsiung, Taiwan; ²Kaohsiung Medical University Hospital, Kaohsiung, Taiwan
- MP 436 **Environmental Exposure to Xenobiotic Agents in Breast Cancer**; Maria Hassis¹; George Lemieux²; Namrata Prasad¹; Susan Fisher¹; Zena Werb²; Katherine Williams¹; ¹Department of Ob/Gyn & Reproductive Sciences, UCSF, San Francisco, CA; ²Department of Anatomy, UCSF, San Francisco, CA
- MP 437 **A Comparative Proteomics Study of Cerebrospinal Fluid from Smith-Lemli-Opitz Syndrome Patients**; Stephanie M. Colonna; Christopher A. Wassif; Sandra K. Conley; Peter S. Backlund; Alfred L. Yergey; Forbes D. Porter; *National Institutes of Health, Bethesda, MD*
- MP 438 **Biomarkers of Dietary Intake to Gauge Health and the Onset of Disease**; Simin D. Maleknia; Russell Bonduri¹; *University of New South Wales, Sydney, Australia*
- MP 439 **Metabolic Profiling of Autistic Brain Tissue Analysis by Laser Ablation Electrospray Ionization**; Rachelle Jacobson; Jessica Stolee; Valerie Hu; Akos Vertes; *George Washington University, Washington, District of Columbia*
- MP 440 **Phosphoproteomics Reveals Activation of FAK Kinase Signaling Pathway in Tamoxifen-Resistant Breast Cancer**; Xinyan Wu¹; Muhammad Zahari¹; Santosh Renuse²; Nandini Sahasrabudhe²; Min-Sik Kim¹; Raghothama Chaerkady¹; Saraswati Sukumar¹; Akhilesh Pandey¹; ¹Johns Hopkins University, Baltimore, MD; ²Institute of Bioinformatics, Bangalore, India
- MP 441 **Down-scaling Tissues Proteomics, toward Precious FFPE Tissue Sample Preparation**; Rémi Longuespée¹; Gabriel Mazzucchelli¹; Nicolas Smargiasso¹; Dominique Baiwir²; Florence Quesada Calvo³; Marie Alice Meuwis³; Philippe Delvenne⁴; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, University of Liège, Belgium; ²GIGA Proteomic Facilities, University of Liège, Liège, Belgium; ³Hepato-Gastroenterology and Digestive Oncology, Liège, Belgium; ⁴Laboratory of Experimental Pathology, Liège, Belgium
- MP 442 **Development of a Diagnostic Proteomic Profiling Platform for Differentiating Thoracic Tumors**; Linan Wang^{1,2}; Konstantin Shilo^{1,3}; Charles Hitchcock^{1,3}; Michael A. Freitas^{1,2}; ¹Ohio State University, Columbus, OH; ²Molecular Virology, Immunology & Medical Genetics, Columbus, OH; ³College of Medicine Pathology, Columbus, OH
- MP 443 **Colorectal Cancer Screening using Targeted LC-MS/MS-Based Metabolic Profiling of Human Serum**; Danijel Djukovic¹; Jiangjiang Zhu¹; Lingli Deng¹; Haiwei Gu¹; Farhan Himmati¹; Gabriela Chiorean^{1,3}; Daniel Raftery^{1,2}; ¹University of Washington, Seattle, WA; ²Fred Hutchinson Cancer Research Center, Seattle, WA; ³Indiana University Melvin and Bren Simon Cancer Ce, Indianapolis, IN
- MP 444 **Discovery of Lipid Biomarkers of Stroke and Cerebral Injury**; Anthony Iavarone¹; Sunil Sheth²; Raymond Swanson^{3,4}; ¹UC Berkeley, Berkeley, CA; ²UCLA, Los Angeles, CA; ³UCSF, San Francisco, CA; ⁴San Francisco Veterans Affairs Medical Center, San Francisco, CA
- MP 445 **Hitting the Target: Novel Reagents for the Chemical-Proteomics Based Identification of Vascular Accessible Biomarkers**; Sabrina Hanke^{1,3}; Alexander Kerner^{1,3}; Yixin Zhang⁴; Christoph Roesli^{1,2}; ¹Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany; ²Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany; ³Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany; ⁴B CUBE Center for Molecular Bioengineering, Dresden, Germany
- Disease Biomarkers, 446 - 467**
- MP 446 **A Glycoprotein Biomarker Panel for Pancreatic Cancer Discovered by Quantitative Mass Spectrometry**; Song Nie¹; Andy Lo¹; Jing Wu¹; Jianhui Zhu¹; Zhijing Tan¹; Diane M. Simeone¹; Michelle A. Anderson²; Kerby A. Shedden³; Mack T. Ruffin⁴; David M. Lubman¹; ¹Surgery department, Ann Arbor, MI; ²Department of Internal, Ann Arbor, Michigan; ³Department of Statistics, University of Michigan, Ann Arbor, Michigan; ⁴Department of Family Medicine, University of Michigan, Ann Arbor, Michigan
- MP 447 **Quantitative Targeted Proteomics-Based Personalized Molecular Target Chemotherapy for Recurrent Brain Tumor**; Sumio Ohtsuki¹; Wataru Obuchi²; Mitsutoshi Nakata³; Jun-ichiro Hamada³; Tetsuya Terasaki²; ¹Kumamoto University, Kumamoto, Japan; ²Tohoku University, Sendai, Japan; ³Kanazawa University, Kanazawa, Japan

- MP 448 **Identification and Comparison of Protein Candidate Biomarkers from Lower Urinary Tract Symptoms (LUTS) in Mouse Models and Human Patients;** Tyler Greer¹; Anatoliy Nechyporenko²; Ling Hao²; Chad Vezina³; Will Ricke⁴; Paul Marker²; Dale Bjorling³; Wade Bushman⁴; Lingjun Li²; ¹Department of Chemistry UW-Madison, Madison, WI; ²School of Pharmacy UW-Madison, Madison, WI; ³School of Veterinary Medicine UW-Madison, Madison, WI; ⁴Department of Urology UW-Madison, Madison, WI
- MP 449 **Targeted and Discovery Proteomic Comparisons of Thyroid Neoplasms Reveals Differential Protein Expression;** Juan Martinez-Aguilar¹; Roderick Clifton-Bligh²; Mark Molloy^{1,3}; ¹Macquarie University, Sydney, Australia; ²Kolling Institute of Medical Research, Sydney, Australia; ³Australian Proteome Analysis Facility, Sydney, Australia
- MP 450 **SRM as a New Efficient Detection Tool for the Early Diagnosis of the Lyme Disease;** Gilles Schnell¹; Amandine Boeuf¹; Benoît Westermann¹; Benoît Jaulhac²; Nathalie Boulanger²; Laurence Ehret-Sabatier¹; ¹LSMBO, Strasbourg, France; ²EA7290, Groupe Borréliose de Lyme, Strasbourg, France
- MP 451 **Detection of Amyloid β -peptides in Cerebrospinal Fluid and Blood Plasma with Immunoprecipitation-MALDI-TOF-MS, using Micropillar Targets on a Silicon Chip;** Johan Jacksén¹; Patrik EK¹; Patrick Öeckl³; Bernd Baumann³; Jens Wiltfang²; Markus Otto³; Johan Roeraade¹; ¹KTH Royal Institute of Technology, Stockholm, Sweden; ²Georg-August-Universität Göttingen, Göttingen, Germany; ³University of Ulm, Ulm, Germany
- MP 452 **Evaluation of Drug Induced Toxicity on Cultured Primary Hepatocytes using MS-based Quantitative Proteomics;** Laxmikanth Kollipara¹; Lisa Dietz¹; Patricio Godoy²; Jan Hengstler²; Albert Sickmann¹; ¹Leibniz-Institut für Analytische Wissenschaften –, Dortmund, Germany; ²Leibniz-Institut für Arbeitsforschung (IfADo), Dortmund, Germany
- MP 453 **Quantitative Profiling of N-linked Glycoproteins from Normal Breast Epithelia and Breast Cancer Cells;** Ten-Yang Yen; Roger Yen; Moe Thein; Yejin Yoo; Alejandro Corona; Judi Wong; Leslie Timpe; Bruce Macher; *San Francisco State University, San Francisco, CA*
- MP 454 **Elevated Peptides in Lung Lavage Fluid Associated with Bronchiolitis Obliterans Syndrome;** Stephen B. Harvey; *University of Minnesota, Minneapolis, MN*
- MP 455 **Analysis of Bone Marrow Derived Multipotent Stromal Cell Secretome** Miljan Kuljanin, David Hess, Gilles A. Lajoie; Miljan Kuljanin; *Western University, London, Canada*
- MP 456 **Systematic Analysis of Tissue Glycoprotein Expression for the Early Detection of Pancreatic Cancer;** Hua Xiao²; Evelyn Kim¹; David Misek¹; ¹University of Michigan, Ann Arbor, MI; ²Shanghai Jiao Tong University, Shanghai, China
- MP 457 **A Combined FASP and TMT Approach (iFASP) for the Identification of CSF Biomarker Candidates for Alzheimer's Disease;** Omar Barnaby^{1,2}; Adam Boxer³; Hanno Steen^{1,2}; Judith Steen^{1,2}; ¹Boston Children's Hospital, Boston, MA; ²Harvard Medical School, Boston, MA; ³University of California, San Francisco, CA
- MP 458 **Characterizing the Nodal-regulated Breast Cancer Secretome and Its Role in Human Bone Marrow Mesenchymal Stem Cell Mediated Tumorigenesis;** Dylan Dieters-Castator¹; Gilles Lajoie¹; Lynne-Marie Postovit²; ¹University of Western Ontario, London, Canada; ²University of Alberta, Edmonton, Canada
- MP 459 **Evaluation of a Protein Marker for Amyotrophic Lateral Sclerosis;** Melinda Beccari¹; Miguel Mitne-Neto²; Valdemir Melechco Carvalho²; Gabriela Venturini³; Mayana Zatz¹; ¹Human Genome and Stem Cell Research Center, São Paulo, Brazil; ²Fleury Group, São Paulo, Brazil; ³Instituto do Coração, São Paulo, Brazil
- MP 460 **High Performance Mass Spectrometry Revealing Phosphorylation-Dependent Regulation of GATA-2 Function;** Chenxi Yang; Koichi Katsumura; Emery Bresnick; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*
- MP 461 **Effect of Fluoride in Insulin Resistance of Gastrocnemium Muscle in Diabetics Rats: A Proteomic Analysis;** Aline Lima Leite^{1,2}; Tatiana Martini¹; Fernanda Zucki¹; Heloísa Aparecida Barbosa da Silva Pereira²; Marília Afonso Rabelo Buzalaf¹; ¹Bauru dental School, Bauru, SP; ²Federal University of São Carlos, São Carlos, SP
- MP 462 **A Sensitive LC/MS/MS Method for the Quantification of Free T3/T4 in Serum, using a Simple Ultrafiltration Sample Preparation Procedure;** Evelyn McClure; *AB SCIEX, Concord, Canada*
- MP 463 **The Role of Proteomics in Deciphering the Intracellular Mechanism of Diuresis by the Insect Vector of Chagas' Disease *Rhodnius prolixus*;** Noman Hassan; Rachit Batta; Paula Gioino; Juan Ianowski; George Katselis; *College of Medicine, University of Saskatchewan, Saskatoon, Saskatchewan, Canada*
- MP 464 **Penile Squamous Cell Carcinoma: Searching for Protein Profiles by Imaging Mass Spectrometry;** Elisângela Silva¹; Adriana Bulgarelli¹; Bernadete Faria²; Isabela Cunha¹; Rafael Rocha¹; Stenio Zequi¹; Gustavo Guimarães¹; Fernando Soares¹; Nilson Assunção²; Jose Vassallo³; ¹AC Camargo Cancer Center, São Paulo, SP-Brazil; ²Federal University of São Paulo, São Paulo, SP-Brazil; ³State University of Campinas Medical School, Campinas, SP-Brazil
- MP 465 **Catalase Corrected Metabolic Syndrome Induced Protein/PTM Changes in a Mouse Model of CVD;** Mark E. Mccomb; Stephen A. Whelan; Chunxiang Yao; Jessica B. Behring; Jean L. Spencer; Christian Heckendorf; Deborah A. Siwik; Wilson S. Colucci; Richard A. Cohen; Markus M. Bachschmid; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- MP 466 **Metabolite Profiling of Foodborne Disease Significance – Case study *Escherichia coli* O157;** Ann Perera¹; Indira Kudva²; Preeti Bais³; Manohar John⁴; ¹Iowa State University, Ames, IA; ²USDA-ARS-NADC, Ames, IA; ³The Jackson Laboratory, Farmington, CT; ⁴Pathovacs Inc, Ames, IA
- MP 467 **Defining Post-Translational Proteolysis Important in Biology and Medicine through N-terminal Labeling;** Reid O'Brien Johnson; Sean Shen; Rachel Ogorzalek Loo; Joseph A. Loo; *University of California, Los Angeles, CA*
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- MP 468 **Identification of Plasmodium Falciparum Thioredoxin Reductase (PfTrxR) Inhibitors from Malaria Box using LC-MS Functional Assay;** Angela Calderon¹; Neil Tiwari¹; Katja Becker²; ¹Auburn University, Auburn, AL; ²Justus Liebig University, Giessen, Germany
- MP 469 **Application of a Molecular Feature Extraction Algorithm to Detect Co-Eluting Species in Degraded Pharmaceuticals;** Fatkhulla K. Tadjimukhamedov; Tsion Billign; Qun Xu; Robyn Powell; Jennifer L. Belsky; John T. Simpson; *United States Pharmacopeia, Rockville, MD*



- MP 470 **Identification of Cooling Agents in Aerosols of an E-Cigarette from Unit Mass Resolution Spectra Enhanced to High Mass Accuracy**; Serban Moldoveanu; Karen Kilby; *Winston-Salem, NC*
- MP 471 **Development of an Ultrafast Screen for Synthetic Cannabinoids using a RapidFire-MS/MS System**; Jennifer Cottine Hitchcock; Ayodele Morris; Gregory McIntire; *Ameritox, Ltd., Greensboro, NC*
- MP 472 **New Approach For Compound Identification using Fine Isotopic Pattern Search**; Caroline Ding¹; Tim Stratton¹; Hans Pfaff²; Hans Gensemann²; Christoph Henrich²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Bremen, Germany*
- MP 473 **Large-Scale Nanoparticle Screening for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry of Plant Metabolites**; Gargey Yagnik^{1,2}; Andrew Korte^{1,2}; Young Jin Lee^{1,2}; ¹*Iowa State University, Ames, IA*; ²*Ames lab US DOE, Ames, IA*
- MP 474 **My ZAB is Dying! Exact Mass Determinations of ESI Invisible Molecules on Qtofs with TAPCI, Toluene Atmospheric Pressure Chemical Ionization**; Todd Williams¹; Larry Seib¹; Robert Drake¹; Jared Mays²; ¹*University of Kansas, Lawrence, KS*; ²*Augustana College, Sioux Falls, SD*
- MP 475 **Small Molecule Analysis using Laser Desorption/Ionization-Mass Spectrometry on Maldi Matrix Incorporated Sol-Gel Film**; Ömür Çelikbıçak; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- MP 476 **Surface Analysis of Permanent Wave Processing Hair using DART-MS**; Shoji Takigami¹; Erika Ikeda¹; Yuta Takagi¹; Jun Watanabe²; Teruhisa Shiota³; ¹*Gunma University, Kiryu, Japan*; ²*Shimadzu Corporation, Kyoto, Japan*; ³*AMR, Inc., Tokyo, Japan*
- MP 477 **Mass Spectrometric Analysis of Oxidation Products generated in an Electrochemical Artificial Kidney**; Maria Viehoff¹; Lars Büter¹; Karin G. F. Gerritsen²; Frank Simonis³; Uwe Karst¹; ¹*University of Muenster, Muenster, D*; ²*University Medical Center Utrecht, Utrecht, The Netherlands*; ³*Nanodialysis B.V., Oirschot, The Netherlands*
- MP 478 **Collision Induced Dissociation Mass Spectra of Protonated Alkyl Dihydrocinnamates**; Sihang Xu; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- MP 479 **Development of a Fast UPLC-MS/MS Screen for Common Drugs of Abuse**; Erin C. Strickland; Gregory McIntire, Ph.D; *Ameritox, Ltd., Greensboro, NC*
- MP 480 **Development of a Qualitative Screen for Select Non-Tricyclic Antidepressants by UPLC/TOF**; Jeremy P. Smith; Erin C. Strickland; Gregory McIntire, Ph.D; *Ameritox, Ltd, Greensboro, NC*
- MP 481 **Software Assisted Rapid Screening and Identification of Potential Genotoxic Degradation Products**; Siji Joseph; Syed Salman Lateed; Vinayak Azhakaprakalam; Sreelakshmy Menon; *Agilent technologies, Bangalore, India*
- MP 482 **Environmental Marker Profiling of Landfill Leachate in Carcass Disposal**; Ryu Ji-Jeong; Seo Jungju; Hwang Geum Sook; *Korea Basic Science Institute(KBSI), Seoul, Korea*
- MP 483 **Characterization of Metabolites of biib028, a Heat Shock Protein 90 Inhibitor, in Rats and Dogs, by High Resolution Mass Spectrometry**; Natalia Penner; Chandra Prakash; *Biogen Idec, Cambridge, MA*
- MP 484 **Identification of Persistent Pd-containing Impurities using LC-MS/MS and LC-ICP-MS**; Wendy Zhong; Qiang Tu; Ryan Cohen; Renee Dermenjian; *Merck, Rahway, New Jersey*
- MP 485 **Avoiding Potential Interferences by Choosing the Right LCMSMS Transition for Midazolam Analysis**; Eric Morin; Jason Bilodeau; Nathalie Pelletier; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 486 **Combined Method for the Analysis of Darunavir, Ritonavir and Lopinavir in Human EDTA Plasma by LCMSMS**; Pierre-Yves Caron; Sylvain Lachance; François Viel; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- MP 487 **A Novel WCX Micro SPE Plate and Its Application in the Sample Extraction for LC-MS/MS Quantitation Method Development**; Guotao Lu¹; Manik Desai²; Dawei Zhou²; Wan Wang³; Jerry Wang¹; ¹*Bonna-Agela Technologies, Inc., Wilmington, DE*; ²*XenoBiotic Laboratories, Inc., Plainsboro, NJ*; ³*Bonna-Agela Technologies, Ltd., Tianjin, China*
- MP 488 **Inhibition of Inter-Conversion between Pitavastatin and its Lactone Metabolite for Application in Clinical Studies using LCMSMS**; Guy Havard; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- MP 489 **Solving Linearity Issue at High Concentration for the Determination of Gemcitabine using LCMSMS**; François Viel; Guy Havard; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Quebec, Canada*
- MP 490 **Highly Selective and Sensitive Determination of Betamethasone-17,21-Dipropionate, Bethamethasone-17-Propionate and Betamethasone by LCMSMS**; Nadia Smith; Philippe Belanger; François Samson-Thibault; Marie-Josée Marcoux; Marie-Claude Theberge; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 491 **Unique Liquid Chromatography Separation of Calcifediol and its 3-epimer analog using Dimethylpentafluorophenyl Propyl Column on a LCMSMS**; Guy Havard; Nicolas Jean; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 492 **Investigation of the Impact of Light on the Determination of Lurasidone in Human Serum by LCMSMS**; Valérie Montminy; Nathalie Pelletier; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 493 **Improved Performance with Column Back-Flushing between Injections: Two Case Studies**; Jason Bilodeau; Nicolas Jean; Marie-Claude Theberge; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 494 **Evaluation of Matrix Effect when Matrix Factor is not Enough for LCMSMS Bioanalytical Method**; Jason Bilodeau; Nadine Lafontaine; Pierre-Yves Caron; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 495 **Resolution of Sildenafil-d8 Ionization Dependence on Sildenafil Concentrations**; Pierre-Yves Caron; Audrey Wilmott; Nancy Lampron; François Viel; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 496 **Lower Limit of Quantitation at Sub-endogenous Compound Level and the Challenge of Low Quality Control Samples Preparation**; Marie-Claude Theberge; Jason Bilodeau; Guy Havard; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*

- MP 497 **Improvement of Sensitivity and Robustness of an LCMSMS Quantitation Method for Digoxin, Controlling the Reactivity of the Deuterated Internal Standard;** Luc Bouchard; Carine Levesque; Nathalie Pelletier; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 498 **Investigation of a Clinical Methodology for Sample Collection for the Determination of Inosine in Human Plasma by LC/MS/MS;** Luc Bouchard; Nathalie Pelletier; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 499 **Quantitative Analysis of Docetaxel in NCR Nude Mice Fat by LC-MS/MS;** Yung-Hsiang Chen; Jason Oeh; Bianca Liederer; Marcel Hop; Brian Dean; Xiao Ding; *Genentech Inc., South San Francisco, CA*
- MP 500 **Application of HILIC Mode to Improve LC/ESI/MS Sensitivity of Opiates and Metabolites;** Anne Mack; William Long; Xiaoli Wang; *Agilent Technologies, Wilmington, DE*
- MP 501 **Stability Investigation on Dimethyl Fumarate in Rat Blood by LC-MS/MS: Insight Into Pharmacokinetics and Metabolic Fate In Vivo;** Venkatraman Junnotula; Hermes Licea Perez; *GSK, King Of Prussia, PA*
- MP 502 **A Highly Selective, Fast and Robust LC/MS/MS Method for the Quantification of Poloxamer 188 in Rat Plasma;** Aihua Liu; Brandon Wilcock; Laixin Wang; Scott Reuschel; Min Meng; *Tandem Labs, Salt Lake City, UT*
- MP 503 **Improving Sensitivity and Throughput for the Quantification of Buprenorphine, Norbuprenorphine, and Naloxone in Human Plasma using LC/MS/MS Assay;** Sherry Liu; Chad Moore; Laixin Wang; Scott Reuschel; Min Meng; *Tandem Labs, Salt Lake City, UT*
- MP 504 **Method Development of a Simultaneous Fast Quantitation of Niacin, Nicotinamide and Nicotinic Acid using HPLC Tandem Mass Spectrometry;** Todd Lusk; *Quintiles Bioanalytical and ADME Labs, Ithaca, NY*
- MP 505 **Challenges on Method Development for the Quantitation of Beclomethasone Dipropionate and Beclomethasone-17-monopropionate in Human Plasma by UPLC@-MS/MS;** Nancy Zheng; Marking G Peay; Michael Waldron; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- MP 506 **Simultaneous Low Level Determination of Ascorbic and Dehydroascorbic Acids using Newly Developed HILIC Stationary Phases and Tandem Mass Spectrometry;** William E. Cotham¹; Audrey M. Howard²; Michael D. Walla¹; Norma Frizzell²; John W. Baynes²; Matthew Przybyciel³; ¹*University of South Carolina, Dept. of Chemistry, Columbia, SC*; ²*University of South Carolina School of Medicine, Columbia, SC*; ³*ES Industries, West Berlin, NJ*
- MP 507 **A General Approach to Eliminating Downfield Interference in Bioanalysis of Amines by SCX Chromatography - Application to Oxybutynin and NNAL;** A Dzerk; P Miller; D Grafelman; E Sarajlic; C Kafonek; *Celerion, Inc, Lincoln, NE*
- MP 508 **Development and Validation of a Rapid and Sensitive LC-MS/MS Method for Quantification of CSUOH0901, an Antitumor Agent;** Ramakrishna Reddy Voggu; Xiang Zhou; Bin Su; Baochuan Guo; *Cleveland State University, Cleveland, Ohio*
- MP 509 **A Novel Derivatization Strategy to Enhance Stability and Sensitivity of LC-MS Detection of Catechol Estrones Extracted from Human Serum;** Lisa Bottalico^{1,2}; Clementina Mesaros^{1,2}; Qingqing Wang^{1,2}; Kannan Rangiah³; Ian A. Blair^{1,2}; ¹*University of Pennsylvania School of Medicine, Philadelphia, PA*; ²*Center for Cancer Pharmacology, Philadelphia, PA*; ³*C-CAMP, Bangalore, INDIA*
- MP 510 **A Single Method for the Quantitation of Sirolimus (Rapamycin) in Whole Blood and Multiple Tissues;** Donald Gray; Tyler DeGraw; Rachel Sun; *BASi, West Lafayette, IN*
- MP 511 **Direct Analysis of Carbodiimides in Pharmaceutical Compounds by High Performance Liquid Chromatography Mass Spectrometry;** Timothy Nowak; Ryan Cohen; Lin Wang; Vincent Antonucci; *Merck, Rahway, NJ*
- MP 512 **Modeling of in vitro Activity with Rat Pharmacokinetics to Remove the Need for in vivo Screening of RIP2 Inhibitors;** Michael Reilly; David Lipshutz; Bart Votta; Helen Sun; Elizabeth Rivera; Mukesh Mahajan; Rakesh Nagilla; Barb Swift; Carol Capriotti; Scott Berger; Linda Casillas; Peter Gough; Robert Marquis; John Bertin; *GlaxoSmithKline, Collegeville, PA*
- MP 513 **A Novel Device for Plasma Micro-Sampling Technique Developed for Bioanalysis;** Ji Zhang; David Lok; Jesse Gray; Matt Jones; *Takeda Pharmaceutical International, Cambridge, MA*
- MP 514 **Method Development and Validation for the Quantitation of ManNAc in Human Plasma using HILIC LC-MS/MS;** Yifan Shi¹; Meng Fang¹; Michael Zhang¹; Yinghe Li¹; Amy Wang²; Ed Kerns²; Nuria Carrillo-Carrasco²; Xin Xu²; Selwyn Yorke³; Bradley Gillespie⁴; ¹*Alliance Pharma, Malvern, PA*; ²*TRND, NCATS, NIH, Rockville, MD*; ³*New Zealand Pharmaceuticals, Palmerston North, New Zealand*; ⁴*Leidos Biomedical Research Inc., Frederick, MD*
- MP 515 **Quantitation and Comparison of A Durg by using Whole Blood Assay and Plasma Assay;** Megan Mimnaugh; John Yu; Jeffrey Duggan; Jennifer Bleecker; Heln Luo; *Boehringer Ingelheim Pharma, Inc., Ridgefield, CT*
- MP 516 **Quantification of Tryptophan and Its Major Kynurenine Metabolites in Human Plasma;** Farid Jahouh; Fang Qian; Rong Wang; *Icahn School of Medicine at Mount Sinai, New York, NY*
- MP 517 **Development of an Ultrasensitive Microflow LC/MS/MS Method for Vitamin D Metabolites Analysis using Amplifex Diene Derivatization Reagent;** Jenny Dai¹; Subhakar Dey²; Eric Battaglioli³; Bruce Stanley¹; Robin Wilson³; ¹*Section of Research Resources, Penn State Univers, Hershey, PA*; ²*AB SCIEX, Chemistry and Consumables R&D, Framingham, MA*; ³*Department of Public Health Sciences, Penn State, Hershey, PA*
- MP 518 **Quantitative Analysis of Microcystins using A Newly Developed Triple Quadrupole Instrument;** Yanan Yang¹; Cindy Tsai²; Anabel Fandino¹; Cameron George¹; Cynthia Hahn¹; ¹*Agilent Technologies, Inc, Santa Clara, CA*; ²*San Jose State University Research Foundation, Gold River, CA*
- MP 519 **Post-column Mobile Phase Adjustment: A Strategy to Eliminate the Contradiction between Liquid Chromatography and Mass Spectrometry in Determining Flavonoids;** Shirui Zheng; *Zhejiang University, Hangzhou, China*
- Homeland Security, 520 - 531**
- MP 520 **Adaptation of U.S. EPA Method 538 Conditions and QC Approach for EA2192 Analysis by Liquid Chromatography/Tandem Mass Spectrometry;** Terry O'Neill¹; Sandip Chattopadhyay²; Stuart Willison³; Matthew Magnuson³; ¹*MRIGlobal, Kansas City, MO*; ²*Tetra Tech, Inc., Cincinnati, OH*; ³*U.S. Environmental Protection Agency, Cincinnati, OH*

- MP 521 **Portable Membrane Inlet Mass Spectrometer for Rapid Detection of Drugs, Explosives and Chemical Weapons;** Stamatios Giannoukos; Boris Brkić; Stephen Taylor; *University of Liverpool, Liverpool, UK*
- MP 522 **Extractive Electrospray Mass Spectrometry of Triacetone Triperoxide Vapour in the Presence of Ionic Liquids;** Alex R. Hill; James C. Reynolds; Martin B. Smith; Paul F. Kelly; Colin S. Creaser; *Loughborough University, Loughborough, UK*
- MP 523 **Detection and Characterization of Chemical Attribution Signatures from Smokeless Powders by Direct Analysis in Real Time – Mass Spectrometry;** Frederick Li¹; Andrew Horsley¹; Joseph Tice²; Brian Musselman²; Adam Hall³; ¹*Boston University School of Medicine, Boston, MA*; ²*IonSense, Inc., Saugus, MA*; ³*Northeastern University, Boston, MA*
- MP 524 **Application of Capillary Atmospheric Pressure Electron Capture Ionization (CAPECI) for the Ultra-Sensitive Detection of Explosives, Drugs and Environmental Toxins;** Valerie Derpmann; David Mueller; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 525 **On-site Identification of Volatile Chemical Warfare Agents by Portable Gas-Chromatography Mass Spectrometry Instrument;** Hisayuki Nagashima¹; Tomohide Kondo¹; Tomoki Nagoya¹; Takeshi Ohmori¹; Mieko Kanamori-Kataoka¹; Kouichiro Tsuge¹; Isaac Ohsawa¹; Yasuo Seto¹; Toru Ikeda²; Naoko Kurimata²; Shohei Unoke²; Manabu Sodeyama³; ¹*National Research Institute of Police Science, Kashiwa, Japan*; ²*INFICON Co., Ltd., Yokohama, Japan*; ³*Teikoku-Sen-i Co., Ltd., Tokyo, Japan*
- MP 526 **On-site Detection of Chemical Warfare Agents by Atmospheric Pressure Chemical Ionization Counterflow-Introduction Ion-Trap Mass Spectrometry with Swab Sampling Mode;** Yasuo Seto¹; Hisayuki Nagashima¹; Tomoki Nagoya¹; Takeshi Ohmori¹; Mieko Kanamori-Kataoka¹; Koichiro Tsuge¹; Isaac Ohsawa¹; Susumu Watanabe²; Hiroaki Hashimoto²; Akihiko Okumura³; ¹*National Research Institute of Police Science, Kashiwa, Japan*; ²*Hitachi High-Tech Solutions Co., Mito, Japan*; ³*Hitachi Ltd., Kokubunji, Japan*
- MP 527 **Multiplex Quantification of Microbial and Plant Protein Toxins in Complex Matrices by Immuno-Extraction And High Resolution Targeted Mass Spectrometry;** Mathieu Dupre¹; Francois FENAILLE¹; Cécile Feraudet-Tarisse¹; Patricia Lamourette¹; Hervé Volland¹; Stéphanie Simon¹; Christophe Junot¹; Virginie Brun²; Francois Becher¹; ¹*CEA, iBiTec-S, SPI, Gif Sur Yvette, France*; ²*CEA, DSV, iRTSV, U1038 INSERM, EDyP, 38054 Grenoble, France*
- MP 528 **Exploration of a Top-Down Absolute Quantification Approach of Staphylococcal enterotoxins by High Resolution Targeted Mass Spectrometry on the Q-Exactive Instrument;** Mathieu Dupre¹; Alexandre Seyer¹; Francois Fenaille¹; Patricia Lamourette¹; Hervé Boutal¹; Hervé Volland¹; Christophe Junot¹; Virginie Brun²; Francois Becher¹; ¹*CEA, iBiTec-S, SPI, 91191 Gif-sur-Yvette, France*; ²*CEA, DSV, iRTSV, U1038 INSERM, EDyP, 38054 Grenoble, France*
- MP 529 **Mass Spectrometric Forensic Analysis of Botulinum Neurotoxin Type A Isolated from Infant Formula and Patient Stool;** Suzanne R. Kalb; Jakub Baudys; John R. Barr; *CDC, Atlanta, GA*
- MP 530 **Optimization of a Mass Spectrometer for Detection of Trace and Bulk Explosives and Narcotics;** Ross Harper; Rakesh Patel; Adam Keil; Mitch Wells; Dennis Barket; *FLIR Systems, West Lafayette, IN*
- MP 531 **Characterization of Analytical Markers in Seized Opium Samples using an Enhanced Ion Mobility Spectrometry-Mass Spectrometry Method;** Peter Liuni¹; Vladimir Romanov²; Marie-Josée Binette³; Hafid Zaknoun³; Maggie Tam³; Pierre Pilon³; Jan Hendrikse²; Derek Wilson¹; ¹*York University, Toronto, ON*; ²*Smiths Detection, Mississauga, ON*; ³*Canada Border Services Agency, Ottawa, ON*
- High Throughput Analysis / Robotics, 532 - 540**
- MP 532 **Evaluation of the SPEware Cerex ALD-III 192 for Use in Automating SPE and SLE Methods in Validated LC-MS/MS Assays;** Patricia L. Holland; Christopher M. Shuford; Martin K. Green; Stacy Dee; Matthew Crawford; Russell P. Grant; *LabCorp, Burlington, NC*
- MP 533 **On-line Automated Protein Precipitation Preparation Followed by LC-MS/MS Analysis and LTD-MS/MS Cross Validation;** Pascal Belisle; Sylvain Letarte; Serge Auger; Pierre Picard; *Phytrox Technologies, Quebec, Canada*
- MP 534 **Automated SAIL on an Orbitrap Exactive;** Andrew Harron¹; Khoa Hoang¹; Milan Pophristic¹; Charles N. Mcewen²; ¹*University of Sciences, Philadelphia, PA*; ²*Univ. of the Sciences, Philadelphia, PA*
- MP 535 **Development and Validation of Direct Analysis Method for Screening and Quantitation of Amphetamines in Urine by LC/MS/MS;** Zhaoqi Zhan¹; Zhe Sun¹; Jie Xing¹; Helmy Rabaha²; Swee Chin Lim²; ¹*Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore*; ²*Department of Scientific Services, Ministry of Health, Brunei Darussalam*
- MP 536 **Mass Spectrometry Based Hit Triage: A Case Study on a Protease using RapidFire Mass Spectrometry;** Junca Meng¹; Gregory Adam¹; Keith Rickert¹; Edward Hudak¹; Ming-Tain Lai²; Jay Grobler²; Paul Zuck¹; Eric Johnson¹; Jeffrey Hermes¹; ¹*Screening and Protein Sciences, Merck Research Lab, North Wales, PA*; ²*Infectious Disease, Merck Research Labs, West Point, PA*
- MP 537 **Investigation of Semi-Automated Serum Processing for High-Throughput N-Glycan Profiling by MALDI-TOF MS;** Yongha In¹; Seounghee Song¹; Jeesu Kim¹; Kyu Hwan Park¹; Yangsun Kim²; ¹*Applied Surface Technology, Suwon, Korea*; ²*Hudson Surface Technology, Old Tappan, NJ*
- MP 538 **High-Throughput Analysis and Characterization of Small and Large Molecules by Matrix Assisted Ionization Vacuum Ion Mobility Spectrometry Mass Spectrometry;** Daniel Woodall; Beixi Wang; Tarick El-Baba; Ellen Inutan; Sarah Trimpin; *Wayne State University, Detroit, MI*
- MP 540 **Utilizing RapidFire Technology Coupled with MS/MS for Label-Free Biochemical Mechanistic Evaluation of Multiple Epigenetic and Metabolism Targets and Inhibitors;** Patrick Bingham; Karen Maegley; Cody Krivacic; *Pfizer, San Diego, CA*
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- MP 549 **Extraction and Molecular Characterization of Water-Soluble Organic Matter in Marine Sediments;** Frauke Schmidt²; Matthias Witt¹; Jens Fuchser¹; Boris P. Koch³; Kai-Uwe Hinrichs²; ¹*Bruker Daltonik GmbH, Bremen, Germany*; ²*MARUM, Bremen, Germany*; ³*AWI, Bremerhaven, Germany*
- MP 550 **Temporal Characterization of Petroleum Residue in Louisiana Salt Marsh Sediments after the Deepwater Horizon Oil Spill by FT-ICR Mass Spectrometry;** Huan Chen¹; Aixin Hou²; Nabanita Bhattacharyya²; Rui Zhang²; Rebecca L. Beasley¹; Ryan P. Rodgers^{1,3}; Alan G. Marshall^{1,3}; Amy McKenna¹; ¹*Nat'l High Magnetic Field Lab, Tallahassee, FL*; ²*Louisiana State University, Baton Rouge, LA*; ³*Florida State University, Tallahassee, FL*

- MP 551 **Rapid Screening and Confirmation Analysis of Polycyclic Aromatic Hydrocarbons (PAHs) with DART Mass Spectrometry;** Yu Takabayashi¹; Jun Watanabe²; Motoshi Sakakura³; Teruhisa Shiota³; ¹SHIMADZU TECHNO-Research, INC., Tokyo, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³AMR, Inc., Tokyo, Japan
- MP 552 **Fast and Automated EPH Fractionation and Clean Up;** Kambiz Sadeghi; Rudolf Addink; *Fluid Management Systems, Watertown, MA*
- MP 553 **Integration of an *in situ* Mass Spectrometer with an Autonomous Underwater Vehicle for Characterization of Dissolved Hydrocarbon Distributions;** Tim Short; Strawn Toler; John Kloske; Steve Untiedt; Mark Ryder; Andres Cardenas-Valencia; Charles Cullins; *SRI International, St Petersburg, FL*
- MP 554 **Molecular Analysis of Aircraft-collected Atmospheric Particles and Cloud Water by nano-DESI and ESI High Resolution Mass Spectrometry;** Eric Boone¹; Alexander Laskin²; Julia Laskin²; Christopher Wirth³; Paul B. Shepson³; Brian Stirm³; Kerri Pratt¹; ¹University of Michigan, Ann Arbor, MI; ²Pacific NW National Laboratory, Richland, WA; ³Purdue University, West Lafayette, IN
- MP 555 **Photochemically-Induced Leaching of Water-Soluble Organics from Macondo Crude Oil into the Environment;** David C. Podgorski^{1,2}; Phoebe Z. Ray³; Huan Chen¹; Amy M. McKenna¹; Ryan P. Rodgers^{1,4}; Alan G. Marshall^{1,4}; Matthew A. Tarr³; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Tallahassee, FL; ³UNO Department of Chemistry, New Orleans, LA; ⁴FSU Department of Chemistry and Biochemistry, Tallahassee, FL
- MP 556 **Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS) for the Real Time, Trace Level Measurement of Naphthenic Acids;** Kyle D. Duncan^{1,3}; Gregory W. Vandergriff¹; Dane R. Letourneau^{1,3}; Dietrich A. Volmer^{1,2}; Erik T. Krogh^{1,3}; Christopher G. Gill^{1,3}; ¹Applied Environmental Research Laboratories (AERL), VIU, Nanaimo, BC, Canada; ²Saarland University, Saarbrücken, Germany; ³Chemistry Department, University of Victoria, Victoria, BC, Canada
- MP 557 **Direct Quantification by Isotope Dilution-Mass Spectrometry of Hydrophobic Analytes Extracted from Wastewater by Stir Bar Sorptive Extraction;** Andrew Boggess; H.M. Skip Kingston; *Duquesne University, Pittsburgh, PA*
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- MP 558 **Systems-Wide Investigation of Photosynthetic Algae during a Shift from Excess- to Limiting- Light Conditions using Multi-Platform Metabolomics and Proteomics;** Nathan Sindt; Graham Peers; Jessica Prenni; *Colorado State University, Ft. Collins, CO*
- MP 559 **A Potential Alternate Synthetic Route to Lignin Thioacidolysis Standards and Their Characterization by GC-MS;** Dawn Kato; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- MP 560 **Elucidation of Synthetic Lignin Oligomers by Tandem Mass Spectrometry;** Fan Huang; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- MP 561 **A GC/MS Procedure for the Rapid Characterization of Algal Liquefaction Products and Process Optimization;** Anna Caldwell¹; Christian Richard²; Bhavish Patel²; John M. Halket^{1,3}; ¹King's College London, London, UK; ²Imperial College London, London, UK; ³Specialist Bioanalytical Services Limited, Egham, UK
- MP 562 **Metaproteogenomic Approaches for Target Discovery of Glycoside Hydrolases and Auxiliary Activities in the Digestome of Lower Termite *Coptotermes gestroi*;** Fabio Squina¹; Macelo Falsarella Carazzolle²; Ana Maria Costa-Leonardo⁴; Ramon Oliveira Vidal²; Gonçalo Guimarães Pereira²; Adriana Franco Paes Leme³; João Paulo Franco Cairo¹; ¹CTBE - CNPEM, Campinas, Brazil; ²UNICAMP, Campinas, Brazil; ³LNBio - CNPEM, Campinas, Brazil; ⁴UNESP, Rio Claro, Brazil
- MP 563 **Effects of Inhibitory Compounds of Lignocellulosic Hydrolysates in Cultivation of Lipid-Producing Bacteria;** Yohannes H. Rezenom; Baixin Wang; Kun-Ching Cho; Janessa L. Tran; Jason Gill; Ryland Young; David H. Russell; Kung-Hui Chu; *Texas A&M University, College Station, TX*
- MP 564 **Profiling of Novel Saponins in Switchgrass using Ultrahigh Performance Liquid Chromatography and Tandem Mass Spectrometry;** Afrand Kamali Sarvestani^{1,4}; Aaron Joseph Garoutte^{2,4}; Leonardo Dacostasousa^{3,4}; Venkatesh Balan^{3,4}; Bruce E Dale^{3,4}; James Tiedje^{2,4}; A. Daniel Jones^{1,4}; ¹Michigan State University Department of Chemistry, East Lansing, MI; ²MSU Department of Microbiology and Molecular Genet, East Lansing, MI; ³MSU Department of Chemical Engineering, East Lansing, MI; ⁴Great Lakes Bioenergy Research Center, East Lansing, MI
- MP 565 **Temporal Resolution and Product Distribution From Glucose to Cellulose using Thin-film Pyrolysis High Resolution Mass Spectrometry;** Daniel Cole; Carolyn Hutchinson; Young Jin Lee; *Iowa State Univ Chemistry Dept, Ames, IA*
- MP 566 **Exploring Molecular Structures using In-source CID on μ Py-GC-APCI-TOF Mass Spectrometry;** Nathan Bond¹; Daniel Cole²; Allison Kvam¹; Carolyn Hutchinson²; Young Jin Lee²; *1*Iowa State University, Ames, IA; *2*Iowa State Univ Chemistry Dept, Ames, IA
- MP 567 **Negative APPI Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Analysis of Fast Pyrolysis Bio-Oils;** Carolyn Hutchinson; Kaitlin Heinen; Young Jin Lee; *Iowa State University, Ames, IA*
- MP 568 **An LC/MS/MS Investigation Of Chemical Reactions Causing Instability in Wood-Derived Pyrolysis Bio-Oils;** Matthew Rasmussen¹; Jincy Joseph²; Brian Frederick²; Elizabeth A. Stemmler¹; ¹Bowdoin College, Brunswick, ME; ²University of Maine, Orono, ME
- MP 569 **Structure and Function of Microbial Communities: Integrating 'Meta-omics' Data Sets;** Eric Huang¹; Frank Aylward²; Paul Piehowski¹; Young-Mo Kim¹; Thomas Metz¹; Cameron Currie²; Stephen Lindemann¹; Margaret Romine¹; William Nelson¹; Jim Fredrickson¹; Richard D. Smith¹; Kristin Kristin Burnum-Johnson¹; Mary Lipton¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²UW-Madison, Madison, WI
- MP 570 **Oxidation of Biodiesel under Electrospray Ionization Process;** Maira Fasciotti¹; Viviane Fernandes da Silva¹; Samantha Ribeiro Campos da Silva¹; Thays Vieira da Costa Monteiro¹; Paulo Roque Martins Silva¹; Werickson Fortunato de Carvalho Rocha¹; Valnei Smarcaro Cunha¹; Romeu José Daroda¹; Marcos Nogueira Eberlin²; ¹INMETRO, Duque De Caxias, Brazil; ²University Of Campinas, Campinas, SP, Brazil
- MP 571 **Metaproteomics and the Ecology of Algal Blooms;** Jags Pandhal; *Sheffield, UK*
- MP 572 **Proteomic and Transcriptomic Analysis of a Solvent Producing Bacterium *Clostridium acetobutylicum* ATCC 824;** Lie Min^{1,2}; Keerthi Venkataraman^{1,2}; Shuyu Hou^{1,2}; E. Terry Papoutsakis^{1,2}; Kelvin H. Lee^{1,2}; ¹University of Delaware, Newark, DE; ²Delaware Biotechnology Institute, Newark, DE

- MP 573 **Advanced MS Analysis of a Novel Biodiesel Production Method**; Derek Waggoner; Patrick Hatcher; *Old Dominion University, Norfolk, VA*
- MP 574 **Small Anhydrooligosaccharides Represent Key Intermediates in Cellulose Fast Pyrolysis**; John Degenstein¹; Priya Murria¹; Matthew Hurt²; James Riedeman¹; Mckay Easton¹; Linan Yang¹; John Nash¹; Rakesh Agrawal¹; W. Nicholas Delgass¹; Fabio Ribeiro¹; ¹*Purdue University, West Lafayette, IN*; ²*Chevron, Richmond, CA*
- MP 575 **Liquid Chromatography/Tandem Mass Spectrometric Method for Quantitative Characterization of Bio-oil from Fast Pyrolysis of Biomass**; Alex Dow; Vinod Kumar Venkatakrishnan; John Degenstein; James Riedeman; Tiffany Jarrell; Christopher Marcum; Ximeng You; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*
- MP 576 **Characterization of Biomass and Biochar by LDI-FTICRMS**; Thierry Ghislain^{1,2}; Vincent Carré³; Yann Le Brech²; Guillaïn Mauviel²; Anthony Dufour^{1,2}; Frédéric Aubriet³; ¹*CNRS, Nancy, France*; ²*Université de Lorraine, Nancy, France*; ³*Université de Lorraine, Metz, France*
- MP 577 **On-Line Mass Spectrometric Analysis of the Primary Fast Pyrolysis Products of Synthetic Lignin Oligomers with β -O-4 and 5-5 Linkages**; Priya Murria¹; Huaming Sheng¹; John Degenstein¹; Weijuan Tang¹; Matthew Hurt²; Ian Klein¹; Hilikka Kenttamaa¹; ¹*Purdue University, West Lafayette, U.S.*; ²*Chevron, Richmond, CA*
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- MP 578 **Sensitivity Increases in Microflow Chromatography for Untargeted Metabolomics in Biomedicine**; Sigurður V. Smárason¹; Jason Causon²; Baldur Bragi Sigurðsson¹; Baljit Ubhi³; ¹*Center for Biomedicine, European Academy Bozen/Bol, Bolzano, Italy*; ²*AB SCIEX, Warrington, UK*; ³*AB SCIEX, Redwood City, CA*
- MP 579 **Development of a Redoxome Platform to Quantify COPD Patient Plasmas for Relative Severity of Oxidative Stress**; Qiuying Chen; Jane Penrose; Ruba Deeb; Crystal Ronald; Steven Gross; *Weill Cornell Medical College, New York, NY*
- MP 580 **Analysis of Metabolites in Human Plasma using GC-TOF MS**; Cristina Di Poto; Yue Luo; Mohammad R Nezami Ranjbar; Rency Varghese; Chi Zhang; Mahlet Tadesse; Habtom Ressom; *Georgetown University, Washington, DC*
- MP 581 **LC-HRMS and Data Mining Tools for the Combined Metabolomic and Lipidomic Serum Profiling of Human Cohorts**; Samia Boudah^{1,2}; Etienne Thévenot³; Alexandre Seyer⁴; Simon Broudin⁴; Lydie Oliveira¹; Florence Castelli¹; Jean-Claude Tabet⁵; Benoit Colsch¹; Christophe Junot¹; ¹*LEMM-CEA-Saclay, Gif-Sur-Yvette, France*; ²*GlaxoSmithKline - Centre de recherche F.Hyafil, Villebon-sur-Yvette, France*; ³*DRT/LIST/DM2/LADIS-CEA-Saclay, Gif-sur-Yvette, France*; ⁴*Profilomic SA, Boulogne-Billancourt, France*; ⁵*LCSOB-UPMC, Paris, France*
- MP 582 **Discriminant Biomarkers of ARDS Associated to H1N1 Influenza Identified by Metabolomics HPLC-QTOF-MS/MS platform**; Alessia Ferrarini¹; Laura Righetti^{1,2}; Francisco J. Rupérez¹; MPaz Martínez¹; Federica Pellati²; José A. Lorente³; Nicolás Nin^{3,4}; Coral Barbas¹; ¹*CEMBIO, San Pablo CEU University, Madrid, Spain*; ²*Università degli Studi di Modena e Reggio Emilia, Modena, Italy*; ³*Hospital Universitario de Getafe, CIBERES, Getafe, Madrid, Spain*; ⁴*Hospital Universitario de Torrejón, Torrejón, Madrid, Spain*
- MP 583 **UPLC-MS Placental Profiling to Investigate Diseases of Pregnancy**; Elizabeth J Want¹; Leanne Nye¹; Julia Langer¹; Catherine Williamson²; Peter Dixon²; ¹*Imperial College, London, UK*; ²*Kings College, London, UK*
- MP 584 **Effect of Ventilation in an Animal Model of Sepsis through a Multiplatform Lung Fingerprinting Approach: From Method Development to Application**; Shama Naz¹; Yeny Rojas²; Leticia Martínez-Caro³; Nicolas Nin⁴; Miguel A. de La Cal²; Antonia García¹; José A. Lorente³; Coral Barbas¹; ¹*CEMBIO, Universidad CEU San Pablo, Boadilla, Madrid, Spain*; ²*Hospital Universitario de Getafe-CIBERES, Madrid, Spain*; ³*H.U. Getafe-CIBERES, Universidad Europea, Madrid, Spain*; ⁴*H.U. Getafe-CIBERES, H.U. de Torrejón, Madrid, Spain*
- MP 585 **Strategies for the Interrogation of Dynamic Exometabolomic Profiles from Mock-Organ Bioreactors**; Cody Goodwin¹; Katrin Zeilinger⁴; Marc Luebberstedt⁴; Ed Darland⁵; Emma Rennie⁵; Rashi Iyer³; Srinivas Iyer³; John Wikswow²; John A. Mclean²; ¹*Vanderbilt Univ Dept of Chem, Nashville, TN*; ²*Vanderbilt University, Nashville, TN*; ³*Los Alamos National Lab, Los Alamos, NM*; ⁴*Charite University, Berlin, Germany*; ⁵*Agilent Technologies, Santa Clara, CA*
- MP 586 **Urinary Metabolomics Analysis Reveals the Impact of the Experimental, Surgical Menopause in Rats**; John Cutts; Stephen Barnes; Landon Wilson; Helen Kim; *University of Alabama at Birmingham, Birmingham, AL*
- MP 587 **Development of a Standard Protocol for High-Throughput Metabolome Profiling of Urine using FIA- and nano-ESI Coupled with FT/ICR-MS**; Baiyi Xue¹; Sandra Alves²; Francois Fenaille³; Benoit Colsch³; Jean-Claude Tabet²; Richard B. Cole²; Alain Paris⁴; Christophe Junot³; Estelle Rathahao-Paris¹; ¹*INRA, AgroParisTech, Équipe IAQA, UMR 1145 Ingéni, Paris, France*; ²*Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*; ³*CEA, iBiTec-S, SPI, Gif Sur Yvette, France*; ⁴*INRA, AgroParisTech, Mét@ risk, Paris, France*
- MP 588 **Metabolomics and Lipidomics Analysis of Murine Plasma and Aortic Tissue in Low Carbohydrate High Protein Diet in Apolipoprotein E-knockout Mice**; Dajana Vuckovic; Mathilde Triguineaux; Olivia Koury; Andreas Bergdahl; *Concordia University, Montreal, Canada*
- MP 589 **A Data-Independent MS/MS Approach to Metabolomics Profiling**; Anne E. Blackwell¹; Mark J. Sartain²; Daniel Cuthbertson³; ¹*Agilent Technologies, Wilmington, DE*; ²*Agilent Technologies, Santa Clara, CA*; ³*Agilent Technologies, Denver, CO*
- MP 590 **Comparative Metabolomics Analyses with IMS-MS Techniques to Determine Molecular Changes in Plasma Upon Exposing Rats to TiO₂ Nanoparticles**; Hossein Maleki; Gregory Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- MP 591 **Comparison of LC/MS Data Processing Methods for Lipidomic Data using MZmine 2.10 and Agilent Profinder**; Stephanie Samra; Brian DeFelice; Ingrid Gennity; Oliver Fiehn; *UC Davis, Davis, CA*
- MP 592 **Metabolomic Studies Reveal that Huntingtin Protein is Essential for Mitochondrial Metabolism, Bioenergetics and Structure in Murine Embryonic Stem Cells**; Steven Gross¹; Qiuying Chen¹; Ismail Ismailoglu¹; Lili Yang¹; Melissa Popowski²; Ali Brivanlou²; ¹*Weill Cornell Medical College, New York, NY*; ²*The Rockefeller University, New York, NY*
- MP 593 **Metabolic Signature of Autism Spectrum Disorders Revealed by High Performance Isotope Labeling LC-MS**; Yiman Wu¹; Chiao-Li Tseng¹; Sidney Tam²; Kelvin SY Leung³; Liang Li¹; ¹*University of Alberta, Edmonton, Canada*; ²*Dept. of Clinical Biochemistry, Queen Mary Hospital, Hong Kong, PR China*; ³*Hong Kong Baptist University, Hong Kong, PR China*

- MP 594 **Metabolomic Analysis of Human Serum using Isotopic Labeling and High-resolution LC-MS for Parkinson's Disease Biomarker Discovery;** Wei Han; Shraddha Sapkota; Richard Camicioli; Roger Dixon; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 595 **Ion Mobility-MS-Based Metabolic Profiling to Distinguish Cancerous and Non-cancerous Breast Tissue Diseases;** Kelly Hines¹; Billy Ballard²; Dana Marshall²; Emma Rennie³; John McLean¹; ¹*Vanderbilt University, Nashville, TN*; ²*Meharry Medical College, Nashville, TN*; ³*Agilent Technologies, Santa Clara, CA*
- MP 596 **Metabolomic Profiling of Anionic Metabolites in Oral Cancer Cells by Capillary Ion Chromatography HR/AM Mass Spectrometry;** Junhua Wang¹; Terri Christison²; Kaori Misuno³; Shen Hu³; Ralf Tautenhahn¹; Linda Lopez²; Yingying Huang¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Sunnyvale, CA*; ³*School of Dentistry and Jonsson Compre. Cancer Ctr, Los Angeles, CA*
- MP 597 **Creation of Reproducible UHPLC-MS/MS Methodology and Compound Libraries for Clinical Metabolomic Applications;** Li Zhang¹; Anna Mathew²; Jaeman Byun¹; Kari Bonds¹; Heidi Baum¹; Sasha Raskind¹; Stephen Brown¹; Charles Burant¹; Subramaniam Pennathur²; ¹*University of Michigan, MRC2, Ann Arbor, MI*; ²*University of Michigan, Department of Internal Med, Ann Arbor, MI*
- MP 598 **Untargeted Metabolomics Reveals that Ascorbic Acid Attenuates Glycerol Trinitrate-Mediated Activation of the (hypo)Xanthine/Xanthine Oxidase System;** Jaewoo Choi¹; Eunice Lee²; Cristobal L. Miranda¹; Jan F. Stevens¹; ¹*Oregon State University, Corvallis, OR*; ²*University of Notre Dame, Notre Dame, IN*
- MP 599 **A Serum Metabolomic *in vitro* Diagnostic Multivariate Index Assay for Prostate Cancer Detection;** Xiaoling Zang¹; Christina Jones¹; Tran Long¹; María Eugenia Monge^{1,2}; Manshui Zhou¹; L. DeEtte Walker¹; Roman Mezencev¹; Alexander Gray¹; John McDonald¹; Facundo Fernández¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*CIBION-CONICET, Ciudad de Buenos Aires, Argentina*
- MP 600 **Metabolomic Study of the Rice Blast Fungus *Magnaporthe oryzae* by GC x GC x QTOFMS;** William Ledford¹; Margarita Marroquin-Guzman¹; Richard Wilson¹; Qingping Tao²; Stephen Reichenbach²; Zhanpin Wu³; Edward Ledford³; Sofia Aronova⁴; Jennifer Gushue⁴; Harry Prest⁴; ¹*University of Nebraska at Lincoln, Lincoln, NE*; ²*GC Image LLC, Lincoln, NE*; ³*Zoex Corporation, Houston, TX*; ⁴*Agilent Technologies, Inc., Santa Clara, CA*
- MP 601 **Examination of Human Serum Samples from Subjects with and without a Chronic Neurodegenerative Disorder;** Jason Winnike¹; Simon Gregory^{1,2}; Xiang Zhang³; ¹*David H. Murdock Research Institute, Kannapolis, NC*; ²*Duke Molecular Physiology Institute, Durham, NC*; ³*University of Louisville, Louisville, KY*
- MP 602 **Optimizing and Benchmarking Untargeted Metabolomics - Quantitative Evaluation of Instrumentation and Methodology to Allow Cross-Lab Comparisons;** Nathaniel G. Mahieu; Amanda Chen; Kevin Cho; Gary J. Patti; *Washington University, St. Louis, MO*
- MP 603 **Effect of Cinnamaldehyde as an Antibacterial Agent on *E. coli* Growth using 96-blade SPME;** Fatemeh Mousavi; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- MP 604 **Global Profiling of *E. coli* Metabolites using Liquid Chromatography- and Gas Chromatography-Mass Spectrometry;** Kelly H. Telu; Nirina R. Andriamaharavo; Ramesh Marupaka; Xinjian Yan; Yamil Simón-Manso; Stephen E. Stein; *NIST, Gaithersburg, MD*
- MP 605 **Untargeted Metabolomics of *Neurospora crassa* Wild Type and the Os-2 Mutant under Heat Shock Stress and 2-deoxyglucose Treatment;** Yuan Xu; Dana M. Freund; Nora Plesofsky; Robert Brambl; Stephen Brockman; Adrian D. Hegeman; Jerry D. Cohen; *University of Minnesota, St. Paul, MN*
- Metabolomics: Identification of Unknown Metabolites, 606 - 630**
- MP 606 **Identification of Unknown Metabolites in *Chlamydomonas reinhardtii* with Accurate Mass GC-QTOF Mass Spectrometry;** John Meissen¹; Kohei Takeuchi²; Zipora Tietel¹; Mine Palazoglu¹; Oliver Fiehn¹; ¹*UC Davis, Davis, CA*; ²*Kao Corporation, Tokyo, Japan*
- MP 607 **Characterization of Metabolites from *Medicago truncatula* using Gas Chromatography High Resolution Time-of-Flight Spectrometry – Knowns and Unknowns;** Jeffrey Patrick¹; Joe Binkley¹; David Alonso¹; David Huhman²; Feng Qiu²; Dennis Fine²; Lloyd W. Sumner²; ¹*LECO Corporation, St. Joseph, MI*; ²*Samuel Roberts Noble Foundation, Ardmore, OK*
- MP 608 **Electron and Chemical Ionization on a Novel GC High Resolution Mass Spectrometer – Tools for the Identification of Unknown Metabolites;** Lorne Fell¹; Jeffrey Patrick¹; Oliver Fiehn²; John Meissen²; ¹*LECO Corporation, St. Joseph, MI*; ²*UC Davis, Davis, CA*
- MP 609 **Targeting and Identifying Trace Metal Metabolites;** Rene Boiteau^{1,2}; Daniel Repeta²; ¹*Massachusetts Institute of Technology, Cambridge, Massachusetts*; ²*Woods Hole Oceanographic Institution, Woods Hole, MA*
- MP 610 **Analysis of Flavonoids from Lotus Leaves by Combining Macroporous Resin Chromatography and LC-MS/MS;** Mingzhi Zhu¹; Lili Jiao²; Wei Wu²; Mingquan Guo^{1,3}; ¹*Wuhan Botanical Garden, Chinese Academy of Science, Wuhan, China*; ²*Changchun University of Chinese Medicine, Changchun, China*; ³*University of Southern California, Alhambra, CA*
- MP 611 **Indole Metabolomics: A Facile Means for the Identification of Indolic Compounds from Plant Tissues;** Peng Yu¹; Janet P. Slovin²; Adrian D. Hegeman¹; Jerry D. Cohen¹; ¹*University of Minnesota, Saint Paul, MN*; ²*USDA/ARS, Beltsville, MD*
- MP 612 **Tracking the Cryptic Biochemistry of Specialized Metabolites in the Medicinal Plant *Camptotheca acuminata* using ¹³C Isotopic Labeling;** Sujana Pradhan; *Michigan State University, East Lansing, US*
- MP 613 **Development of Compound Identification Technique for Conjugated Unknown Compounds using Ion Trap Time-of-Flight Mass Spectrometry;** Tairo Ogura^{1,2}; Akihiro Tai³; Takeshi Bamba²; Eiichiro Fukusaki²; ¹*Shimadzu corporation, Kyoto, Japan*; ²*Osaka University, Osaka, Japan*; ³*Prefectural University of Hiroshima, Hiroshima, Japan*
- MP 614 **Development of Tandem Mass Spectral Libraries for Plant Metabolomics and Metabolite Identifications;** Dennis D. Fine¹; Feng Qiu¹; Sandy Yates²; Romano Hebel³; Aiko Barsch³; Lloyd W. Sumner¹; ¹*Plant Biology Division, The Noble Foundation, Ardmore, OK*; ²*Bruker Daltonics, Fremont, CA*; ³*Bruker Daltonics, Bremen, Germany*
- MP 615 **Mass Spectral Based Strategies for Rapid Identification of Novel Metabolites Unraveling Evolutionary Patterns of HGL-DTG Biosynthesis in the genus *Nicotiana*;** Sven Heiling¹; Emmanuel Gaquerel²; Aiko Barsch³; Arnd Ingendoh³; Ian T. Baldwin¹; ¹*Max Planck Institute for Chemical Ecology, Jena, Germany*; ²*Centre for Organismal Studies Heidelberg, Heidelberg, Germany*; ³*Bruker Daltonik, Bremen, Germany*

- MP 616 **Structural Characterization and Fragmentation Rule Generation of Flavonoids using Fragmentation Trees;** Arpana Vaniya; Yan Ma; Tobias Kind; Oliver Fiehn; UC Davis, Davis, CA
- MP 617 **De novo Metabolite Identification in the Soil Bacterium *Acinetobacter baylyi* ADP1 using H/D Exchange, ESI/HRMS and MSⁿ;** Lucille Stuani¹; Christophe Lechaplais¹; Ekaterina Darii¹; Marcel Salanoubat¹; Alain Perret¹; Jean-Claude Tabet²; ¹CEA-Genoscope/UMR8030, Evry, France; ²UPMC-IPCM/CSOB/UMR7201, Paris, France
- MP 618 **Structure Elucidation of Novel Natural Products of Streptomycetes by Molecular Networking and Ion-Mobility Spectrometry;** Andrew R. Johnson¹; Chan Gao²; Marie Elliott²; Erin E. Carlson¹; ¹Indiana University, Bloomington, IN; ²McMaster University, Hamilton, ON, Canada
- MP 619 **LC-TOF MS Profiling of Glutathione Conjugates of Endogenous Oxylipins in *Arabidopsis* leaves;** Jiangyin Bao; A. Daniel Jones; Michigan State University, East Lansing, MI
- MP 620 **The Electrochemical Simulation of Selegiline Metabolism Leads to Generation of Amphetamines;** Przemyslaw Mielczarek¹; Marek Smoluch¹; Krzysztof Labuz²; Piotr Suder¹; Jerzy Silberring^{1,3}; ¹AGH University of Science and Technology, Krakow, Poland; ²The Rydygier Hospital, Addiction Outpatient Clinic, Krakow, Poland; ³Centre of Polymer and Carbon Materials, PAN, Gliwice, Poland
- MP 621 **Mapping Distribution of Sulfur-containing Metabolites in Health-promoting Crops by S-omics using Ultrahigh Performance Mass Spectrometry;** Ryo Nakabayashi¹; Kazuki Saito^{1,2}; ¹RIKEN Center for Sustainable Resource Science, Yokohama, Japan; ²Chiba University, Chiba, Japan
- MP 622 **Cyclic Peptide Substructures Automatically Assigned using Exact Mass ESI/MSMS Data and the MASSPEC Algorithm;** Marshall M. Siegel¹; Gary Walker¹; Eugene Ciccimaro²; Serhiy Hnatyshyn²; ¹MS Mass Spec Consultants, Fair Lawn, NJ; ²Bristol-Myers Squibb, Lawrenceville, NJ
- MP 623 **Addressing Identification Ambiguity in Untargeted Metabolomics by Processing Raw Spectra into a High Quality Reference Data;** Juraj Lutisan¹; Yingying Huang²; Mark Sanders²; Eric Genin³; Robert Mistrik¹; ¹HighChem, Bratislava, Slovakia; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Villebon sur Yvette, France
- MP 624 **iElement: New UHRMS Signal Handling Approach for More Accurate Elemental Composition Determination;** Wei-Hung Chang¹; Yu-Chen Huang¹; Han-Jia Lin²; Yet-Ran Chen¹; ¹Academia Sinica, Taipei, TAIWAN; ²National Taiwan Ocean University, Keelung, Taiwan
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- Somang Kim¹¹; Kevin Bateman¹¹; ¹Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; ²AbbVie, Ludwigshafen, Germany; ³Biogen Idec, Cambridge, MA; ⁴Bristol-Myers Squibb Company, Wallingford, CT; ⁵Bruker, Billerica, MA; ⁶F. Hoffmann-La Roche Ltd, Basel, Switzerland; ⁷Pfizer Inc., Groton, CT; ⁸Pompeu Fabra University, Barcelona, Spain; ⁹University of Perugia, Perugia, Italy; ¹⁰Merck Research Labs, Kenilworth, NJ; ¹¹Merck & Co., West Point, PA
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- MP 642 **Swath MSMS: Smart Data Acquisition Workflows for Metabolite Identification;** Natalia Penner¹; Suma Ramagiri²; Chandra Prakash¹; ¹Biogen Idec, Cambridge, MA; ²AB SCIEX, Concord, ON
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- MP 651 **Fast Ion Mobility Spectrometry and High Resolution TOF MS;** Boris Kozlov¹; Vasily Makarov¹; Igor Kurnin²; Anatoly Verenchikov¹; ¹MS Consulting, Bar, Montenegro; ²Institute for Analytical Instrumentation, RAS, St. Petersburg, Russia
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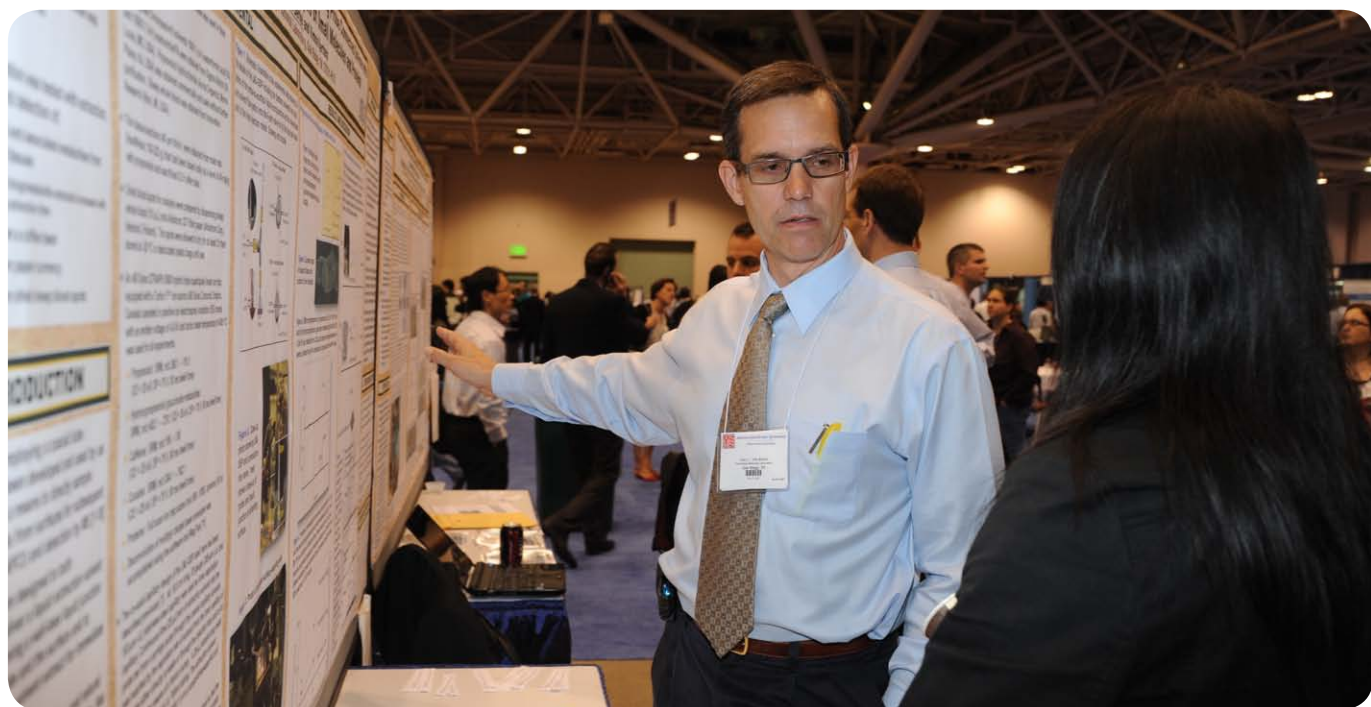
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- MP 709 **Identification and Quantification of Electrochemically Generated Metabolites of Thyroxine (T4) by Means of LC-ESI-MS and LC-ICP-MS with Counter Gradient Elution**; Chun Kong Mak^{1,2}; Christoph A. Wehe¹; Michael Sperling^{1,3}; Uwe Karst¹; ¹University of Muenster, Muenster, Germany; ²NRW Graduate School of Chemistry, Muenster, Germany; ³EVISA, Muenster, Germany
- MP 710 **Maximizing Nanoflow Spray Stability and Sensitivity using Automated Emitter Rinsing**; Amanda Berg; Helena Svobodova; Gary A. Valaskovic; *New Objective, Inc., Woburn, MA*
- MP 711 **Validation of an In-Source Micro Flow LC-MS/MS Method for Bioanalysis**; Casey Johnson; Chad Christianson; Shane Needham; Sharon DeChenne; *Alturas Analytics, Moscow, ID*
- MP 712 **Continuous Sampling System for Liquid Chromatography-Mass Spectrometry-Based Detection of Intact Proteins and Small Molecules**; Kendra R. Evans; Braydon L. Dymm; Dominick J. Alton; *University of Detroit Mercy, Detroit, U.S.*
- MP 713 **Preparative Two Dimensional LC-SFC/MS Techniques for the Purification of Organic Compounds from the Complex Mixtures**; Zahid Ali; Mary Ababat; Lu Zeng; *Takeda California, San Diego, CA*
- MP 714 **Applications of Supercritical Fluid Chromatography for Chiral Metabolite Separations in a DMPK Bioanalytical Laboratory**; Hermes Licea Perez¹; Dana Knecht¹; Christopher Evans¹; Mark Wrona²; Paul Rainville²; ¹Bioanalysis / GSK, King Of Prussia, PA; ²Waters, Milford, MA
- MP 715 **A Novel Hybrid SFC/UHPLC/MS System Optimized for Low Peak Dispersion**; Patric Hoerth¹; Rick Wikfors²; Tom A. van de Goor¹; ¹Agilent Technologies R&D, Waldbronn, Germany; ²Agilent Technologies, Toughkenamon, PA
- MP 716 **Intelligent Algorithm for Multidimensional Optimization of Time of Flight Instrumentation**; Javier Satulovsky; Huy Bui; Brian Smart; William Frazer; Maithilee Samant; George Stafford; Gregor Overney; *Agilent Technologies, Santa Clara, CA*
- MP 717 **Exploring the Uncharted Depths of the Complex Human Proteome using the Orbitrap Fusion Mass Spectrometer**; Graeme Mcalister; Jesse D. Canterbury; Philip M Remes; Shannon Eliuk; Vlad Zabrouskov; Michael W. Senko; *Thermo Fisher Scientific, San Jose, CA*
- MP 718 **Q-Exactive Plus and Orbitrap Fusion: Determination of Optimal Settings for Peptide and Phosphopeptide Identification**; Thiago Verano-Braga; James Williamson; Alistair Edwards; Ole Nørregaard Jensen; Frank Kjeldsen;

- Martin Røssel Larsen; *University of Southern Denmark, Odense, Denmark*
- MP 719 **Qualitative and Quantitative Comparison of Q Exactive Plus and Orbitrap Fusion for Label Free and Isobaric Tag Based Quantification;** James Williamson; Thiago Verano-Braga; Alistair Edwards; Ole Nørregaard Jensen; Frank Kjeldsen; Martin Røssel Larsen; *University of Southern Denmark, Odense, Denmark*
- MP 720 **Robustness Study of Peptides in Plasma using Novel Technologies in an LC-MS Instrument;** Karen Salomon; Maurizio Splendore; Louis Maljers; Zicheng Yang; Steven Schachterle; *Bruker, Fremont, CA*
- MP 721 **Extending Inter Scan Linear Dynamic Range on a QqTOF platform;** Feng Zhong; Doug Simmons; J.C. Yves Leblanc; Nic Bloomfield; *AB SCIEX, Concord, On, Canada*
- MP 722 **Electron Ionization in LC-MS: Increasing Selectivity and Sensitivity;** Achille Cappiello¹; Hanno Evard²; Giorgio Famiglioni¹; Pierangela Palma¹; Veronica Termopoli¹; ¹*University of Urbino, Urbino, Italy*; ²*University of Tartu, Tartu, Estonia*
- MP 723 **Improved Sensitivity for Shotgun Proteomics on an ES TOF Instrument through a Combination of Acetonitrile Dopant and Zero Dead-Volume CaptiveSpray;** Scarlet Beck¹; Igor Paron¹; Annette Michalski²; Stephanie Kaspar²; Markus Lubeck²; Carsten Baessmann²; Juergen Cox¹; Matthias Mann¹; ¹*Max Planck Institute of Biochemistry, Martinsried, Germany*; ²*Bruker Daltonik GmbH, Bremen, Germany*
- MP 724 **Coupling Laser Ablation Sample Transfer and LC-ESI-MS for tissue imaging;** Fabrizio Donnarumma; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- MP 725 **Capillary Exit Voltage-Induced vs. CID Fragmentation Behavior of Four Antiviral Drugs in an Agilent Ion Trap Mass Spectrometer;** Mohamed W Attwa; Nasser Salem; Ali S. Abdelhameed; A. F. M. Motiur Rahman; Adnan A. Kadi; *King Saud University, Riyadh, Saudi Arabia*
- MP 726 **A Comparative Study of Chalcones Fragmentation: Induced In-source Fragmentation in ESI-Triple Quadrupole with MS3 in ESI-Ion Trap;** Adnan A Kadi; Mohamed W. Attwa; A. F. M. Motiur Rahman; *King Saud University, Riyadh, Saudi Arabia*
- LCMS Chromatography, 727 - 752**
- MP 727 **Spectroscopic Investigation in Differentiating Random from Block Polyether Copolymers using Reversed-Phase LC Coupled with ELSD or MS;** Robielyn Ilagan; Shenmin Pan; Ernest Long; *MacDermid Electronics Solutions, Waterbury, CT*
- MP 728 **Combining Mass Spectra with UV Spectra for Orthogonal Chromatographic Detection and Peak Identification;** Thomas E. Wheat¹; Aparna Chavali²; Sean McCarthy²; Paula Hong²; Patricia McConville²; ¹*Waters Corporation, Hopedale, MA*; ²*Waters Corporation, Milford, MA*
- MP 729 **Routine MS Detection Applied to USP Chromatographic Methods;** Thomas E. Wheat¹; Daniel Root²; Aparna Chavali²; Patricia McConville²; ¹*Waters Corporation, Hopedale, MA*; ²*Waters Corporation, Milford, MA*
- MP 730 **Applicability of novel Supercritical Fluid Chromatography Tandem Quadrupole-Time of Flight Mass Spectrometry;** Jianzhong Li; Ying Meng; Tao Bo; Rong An; *Agilent Technologies(China), Beijing, China*
- MP 731 **Coupling of HPLC with ESI-MS for Studying the Aging of Ultrasmall Multimodal Nanoparticles;** Charles Truillet; François Lux; Olivier Tillement; Philippe Dugourd; Rodolphe Antoine; *Institut Lumière Matière, UMR5306 Université Lyon, Villeurbanne, France*
- MP 732 **Sensitivity of Detection of 12 Aminoglycoside Antibiotics by Positive ESI – Comparison between HILIC and Reverse Phase Methods;** Olga Shimelis; Emily Barrey; Dave Bell; Craig Aurand; *Sigma-Aldrich, Bellefonte, PA*
- MP 733 **Orthogonal Fast and Ultra-Fast Reverse Phase Chiral LC/MS Methods for the Analysis of Stereoisomeric Pharmaceutical Compounds;** Alfonso Espada; Cristina Anta; *Lilly S.A., Alcobendas, Spain*
- MP 734 **Improved LC-MS/MS Method for the Quantitation of the Plant Hormones Abscisic Acid and Indole-3-Acetic Acid;** Yongxin Nie¹; Yinggao Liu¹; Hongxia Jiang¹; Ron Orlando²; ¹*ShanDong Agricultural University, Taian, SD*; ²*University of Georgia, Athens, GA*
- MP 735 **Development of a Sensitive LC/MC/MS Assay for the Analysis of Total Testosterone and Steroids in Human Serum;** Liming Peng¹; Cheni Krishnan²; Eric Davis²; Xiaohong Chen¹; Bhasin Shalender¹; ¹*Brigham and Women's Hospital, Boston, Massachusetts*; ²*AB Sciex, Foster City, CA*
- MP 736 **The Application of Multiple LC/MS Methods to Help Determine the m/z of a Low Level Impurity in a Drug Product;** Wendy Hengwen Zhong; Michael Matchett; Randy Wilhelm; *Mallinckrodt, Saint Louis, MO*
- MP 737 **Selection of Negative Mode Standard in LC-MS under Neutral Condition for Assessing Solvent Quality;** Subhra Bhattacharya; Deva H. Puranam; Stephen C. Roemer; *Thermo Fisher Scientific, Fair Lawn, NJ*
- MP 738 **Improved Automated Reversed-Phase HPLC-MS Methods for Quantitative Amino Acid Analysis;** Keely Glass¹; Jen Skeritt¹; Carol Jiang¹; Roman Lin¹; George Dubai¹; Amy Huang¹; John Simon^{1,2}; ¹*Duke University, Durham, NC*; ²*University of Virginia, Charlottesville, VA*
- MP 739 **Analysis of D- and L-amino Acids using Automated Pre-Column Derivatization and Liquid Chromatography-Electrospray Ionization Mass Spectrometry;** Kenichiro Tanaka¹; Hidetoshi Terada²; Yoshiko Hirao²; Kiyomi Arakawa²; Yoshihiro Hayakawa²; ¹*Shimadzu Scientific Instruments, Inc., Columbia, MD*; ²*Shimadzu Corporation, Kyoto, Japan*
- MP 740 **Development of a Novel Amino Acids Analysis Column for LC-MS without Derivatization;** Itaru Yazawa; Hiroshi Tachikawa; *Imtakt Corporation, Kyoto, Japan*
- MP 741 **LC-MS Analysis of "Dirty" Food and Pharma Samples with Monolithic Silica Columns;** Stephan Altmaier; Egidijus Machtejevas; Karin Cabrera; *Merck Millipore, Merck KGaA, Darmstadt, Germany*
- MP 742 **Full Optimization of LCMS Methods to Increase Robustness of Complicated Matrix Containing Samples using Active Flow Management Chromatography;** Eric Stover¹; Mark Dreyer¹; Mary Blackburn¹; Luisa Pereira²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Runcorn, Cheshire, UK*
- MP 743 **Analyzing Highly Organic Samples, Polar Analytes, and Large Volume Injections using Microflow Chromatography Coupled with Mass Spectroscopy;** Subodh Nimkar¹; Khaled Mriziq¹; Leo Wang²; ¹*SCIEX Separations, Division of AB SCIEX, Redwood City, CA*; ²*AB SCIEX, Redwood City, CA*
- MP 744 **Fabrication of Stage-Frit NanoLC column for Proteomic Analysis;** Ming-Yueh Hsieh; He-Hsuan Hsiao; *NCHU, Department of Chemistry, Taichung, Taiwan*
- MP 745 **Advancing Host Cell Protein Analyses through Improved Microscale Peptide Separations and 2D UHPLC Chromatography;** Matthew Lauber; Catalin Doneanu; Stephan Koza; Weibin Chen; Kenneth Fountain; *Waters Corporation, Milford, MA*

- MP 746 **Design and Evaluation of a Modified Salt Pulse Scheme for Increased Measurement Depth in a MudPIT Proteome Experiment;** Ramsunder Iyer^{1,2}; Richard J. Giannone¹; Robert Hettich¹; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*; ²*University of Tennessee, Knoxville, TN*
- MP 747 **Finding the Appropriate LC Setup for Proteomics Experiments Depending on the Sample Complexity using Chip-Based Columns;** Jan Muntel¹; Helena Svobodova²; Gary A. Valaskovic²; Saima Ahmed¹; Kevin Broadbelt¹; Omar Barnaby¹; Hanno Steen¹; ¹*Boston Children's Hospital, Boston, MA*; ²*New Objective, Woburn, MA*
- MP 748 **Improved Protein Identification by nanoLC/MS/MS using Chip Based Columns with Integrated Post-Column Addition of DMSO for Increased Sensitivity;** Remco van Soest¹; Christie Hunter²; Hao Yang¹; ¹*Sciex Separations, Redwood City, CA*; ²*AB SCIEX, Redwood City, CA*
- MP 749 **Normal Phase LC/MS Post Additive Infusion for Vitamin D3 EP Method 01/2013:0072 With No LC Modifications;** Keith Rippel; *Pfizer Consumer Healthcare, Richmond, VA*
- MP 750 **Enhancing MS Sensitivity in Negative Electrospray Mode by Post-Column Addition of a Modifier;** Angela Doneanu¹; James Murphy²; ¹*Waters, Milford, MA*; ²*Waters Corporation, Milford, MA*
- MP 751 **Optimization of Intact Protein RP-LC-MS Analysis using a Characterized Standard Protein Mix;** Benjamin Cutak; Jim Blasberg; Gordon Nicol; Kevin Ray; *Sigma-Aldrich, Saint Louis, MO*
- MP 752 **Assessment of the Effects of Intact Protein Mass Measurements by On-Line Liquid Chromatography Coupled with Mass Spectrometry;** Jinghua Zhu; Qishan Lin; *State University of New York at Albany, Rensselaer, NY*
- LCMS Sample Preparation I (Drugs and Metabolites), 753 - 786**
- MP 753 **Automating On-Line Extraction, Derivatization and Cleanup with LC-MS to Measure Estrogens in Biological Fluids;** Jennifer Poshkus¹; Heather Heilman¹; Joseph Di Bussolo²; ¹*West Chester University of Pennsylvania, West Chester, PA*; ²*Thermo Fisher Scientific, West Chester, PA*
- MP 754 **LC-MS/MS with Novel Online Cleanup Valving Solution for Quantitative Analysis of Testosterone in Serum;** Andre Szczesniowski; Sheher Bano Mohsin; *Agilent Technologies, Schaumburg, IL*
- MP 755 **Analysis of Vitamin D3 in Dietary Supplements by 2-dimensional LC System;** Taku Tsukamoto; Kazuhiro Sonomura; Keiko Yamabe; Kiyomi Arakawa; Yoshihiro Hayakawa; *Shimadzu Corporation, Kyoto, Japan*
- MP 756 **A Reduced Workflow Method for the Extraction of Vitamin B7 from Human Serum with No Drydown Prior to Mixed-Mode LC-MS/MS;** Frank Kero; Victor Vandell; Lee Williams; Geoff Davies; Adam Senior; Rhys Jones; Helen Lodder; Elena Gairloch; Claire Desbrow; Wendy Hartsock; *Biotage, Charlotte, NC*
- MP 757 **Comparison of SPE Approaches for the Extraction of Thyroid Hormones: T3, rT3 and T4 prior to LC-MS/MS Analysis;** Lee Williams¹; Helen Lodder¹; Adam Senior¹; Rhys Jones¹; Alan Edgington¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Victor Vandell²; Frank Kero²; ¹*Biotage GB Limited, Cardiff, UK*; ²*Biotage LLC, Charlotte, NC*
- MP 758 **Supported Liquid Extraction of Vitamin D Metabolites: 25-hydroxy and 1 α ,25-dihydroxy Vitamin D₂/D₃ using PTAD Derivatization Prior to LC-MS/MS Analysis;** Rhys Jones¹; Alan Edgington¹; Lee Williams¹; Adam Senior¹; Helen Lodder¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Victor Vandell²; Frank Kero²; ¹*Biotage GB Limited, Cardiff, UK*; ²*Biotage LLC, Charlotte, NC*
- MP 759 **Vitamin D Metabolites in Serum: Extraction using Phospholipid Depletion Technology (PLD) Prior to UPLC-MS/MS Analysis;** Victor Vandell¹; Lee Williams²; Alan Edgington²; Frank Kero¹; Elena Gairloch¹; Rhys Jones²; Adam Senior²; ¹*Biotage, Charlotte, NC*; ²*Biotage GB Limited, Cardiff, N/A*
- MP 760 **Extraction of Antiepileptic Drugs from Biological Fluids using Supported Liquid Extraction (ISOLUTE® SLE+) in 96-Well Plate Prior to LC-MS-MS Analysis;** Victor Vandell¹; Frank Kero¹; Elena Gairloch¹; Lee Williams²; Adam Senior²; Rhys Jones²; Geoff Davies²; Alan Edgington²; ¹*Biotage, Charlotte, NC*; ²*Biotage GB Limited, Cardiff*
- MP 761 **Extraction of Mycophenolic Acid and Mycophenolic Acid Metabolite from Serum using Supported Liquid Extraction Prior to LC-MS-MS Analysis;** Victor Vandell¹; Frank Kero¹; Elena Gairloch¹; Lee Williams²; Adam Senior²; Rhys Jones²; Geoff Davies²; Alan Edgington²; Martin Cherrier¹; ¹*Biotage, Charlotte, NC*; ²*Biotage GB Limited, Cardiff, N/A*
- MP 762 **Single Step Separation of Plasma from Whole Blood without the Need for Centrifugation Applied to the Quantitative Analysis of Warfarin;** Alan J Barnes¹; Adam McMahon²; Neil J Loftus¹; ¹*Shimadzu, Manchester, UK*; ²*WMIC, University of Manchester, Manchester, UK*
- MP 763 **Fully Automated Analysis of Immunosuppressant Drugs with ZinMass-200 Clinical LC-MS/MS Analyzer;** Murat Celik; Huseyin Avni Cavdar; *ZIVAK Technologies, Istanbul, Turkey*
- MP 764 **Challenges and Strategies in Developing an Ultrafiltration/LC/MS/MS Assay for Quantitation of Unbound Paclitaxel in Human Plasma Following Abraxane Treatment;** Linge Li; Michael P. Waldron; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- MP 765 **Troubleshooting of Low Recovery of LC-MS Method for 2-Hydroxypyridine-N-oxid (HOPO) in a Drug Candidate Substance during Technical Transfer;** Gang Tang; Qinggang Wang; Peter Tattersal; *Bristol-Myers Squibb, New Brunswick, NJ*
- MP 766 **Removal of Phospholipids using Phosphate-Selective Sorbent;** Chiaki Aoyama; Shigenori Ota; Yuko Yui; Kosuke Osaka; Masakazu Takahashi; Masayoshi Ohira; *GL Sciences Inc., Shinjuku-Ku, Japan*
- MP 767 **Extraction of Telmisartan from Human Plasma using an Improved Capacity Supported Liquid Extraction (SLE) 96-well Plate;** Matthew Cleeve; Tina Ovitt; *Kinesis, St Neots, UK*
- MP 768 **Extraction of Indomethacin and Ibuprofen from Small Volume Biological Fluid Samples using a New Versatile μ Elution SPE 96-well Plate Format;** Matthew Cleeve; *Kinesis, St Neots, UK*
- MP 769 **Quantification of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL) in Urine using Solid-Phase Extraction and UPLC-ES/MS/MS;** Kellie Woodling¹; Frank Kero²; Victor Vandell²; Goncalo Gamboa da Costa¹; ¹*NCTR, Jefferson, AR*; ²*Biotage, Charlotte, NC*
- MP 770 **High-Throughput SPME-UPLC-MS as a Convenient Method for the Simultaneous Determination of Various Prohibited Substances in Urine and Plasma;** Nathaly Reyes-Garcés; Ezel Boyaci; Krzysztof Gorynski; Ángel Rodríguez-Lafuente; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- MP 771 **A New Approach to Automated Method Development for LC-MS/MS Sample Preparation;** Guy Burssens¹; Roland Geyer¹; Jeffrey Enders²; ¹*Tecan, Männedorf, Switzerland*; ²*Ameritox, Ltd., Greensboro, TN*



- MP 772 **Automated Hydrolysis, DPX Extraction and LC/MS/MS Analysis of Pain Management Drugs from Urine;** Fred Foster¹; Oscar Cabrices¹; John Stuff¹; Edward Pfannkoch¹; William Brewer²; ¹Gerstel, Inc., Linthicum, MD; ²University of South Carolina, Columbia, SC
- MP 773 **Utilizing Beta Glucuronidase Enzymatic Digest for LC/MS Analysis for Glucuronide Metabolites;** Craig Aurand; Dave Bell; Emily Barrey; Olga Shimelis; *Sigma Aldrich, Bellefonte, PA*
- MP 774 **Aminoglycoside Analysis in Pork Muscle using Molecularly Imprinted Polymer Cleanup and LC-MS/MS Detection;** Emily Barrey; Olga Shimelis; Carmen Santasania; Xiaoning Lu; *Sigma-Aldrich, Bellefonte, PA*
- MP 775 **Identification and Quantification of Lignin Degradation Products in Highly Saline Mixtures by Two-Stage HPLC Coupled with ESI Tandem Mass Spectrometry;** Hanyu Zhu¹; Christopher Marcum¹; Christopher Gulvik²; Alison Buchan²; Hilikka Kenttämä¹; ¹Purdue University, West Lafayette, IN; ²University of Tennessee, Knoxville, TN
- MP 776 **A New Fully Automated Online SPE/HPLC-MS/MS Method for the Determination of Phenoxycarboxylic Acids in Water;** Franziska Chmelka¹; Oscar Cabrices²; Edward Pfannkoch²; ¹Labor Dr. Helle GmbH & Co.KG, Bremerhaven, Germany; ²Gerstel Inc., Linthicum, MD
- MP 777 **Simplified Dioxin Sample Preparation using a Novel Carbon Adsorbent;** Dr. Conor Smith; *United Science Corp, Minneapolis, MN*
- MP 778 **Removing Phthalate Contamination from Organic Solvents using a Novel Carbon Sorbent;** Doug Fryer; *United Science Corp, Minneapolis, MN*
- MP 779 **New Solvent Grade Targeted for Trace Analysis by UHPLC-MS;** Subhra Bhattacharya; Deva H. Puranam; Stephen C. Roemer; *Thermo Fisher Scientific, Fair Lawn, NJ*
- MP 780 **Aminopyrene and Aminopyrene-based GUMBOS as Novel Matrices for MALDI-MS;** Hashim Alghafly; Kermit K. Murray; Isiah M. Warner; *Baton Rouge, LA*
- MP 781 **Bioanalytical Considerations for Utilizing a Capillary Micro-sampling Device for Plasma Collection and Isolation with LC-MS Detection;** Sharon Boram¹; Chester L Bowen¹; Jim Kenney²; Joseph Siple²; ¹GlaxoSmithKline, King Of Prussia, PA; ²Drummond Scientific, Broomall, PA
- MP 782 **A Simplified Load-Wash-Elute Solid Phase Extraction Protocol for the Oasis® HLB µElution Plate;** Xin Zhang; Pamela Iraneta; Frank Marszalkowski; *Waters Corp, Milford, MA*
- MP 783 **Evaluation of a Novel 96-well Filter Plate for the Effective Removal of Serum Protein and Phospholipids prior to LC-MS/MS Analysis;** Lee Williams¹; Helen Lodder¹; Geoff Davies¹; Steve Plant¹; Adam Senior¹; Alan Edgington¹; Rhys Jones¹; Steve Jordan¹; Claire Desbrow¹; Victor Vandell²; Frank Kero²; ¹Biotage GB Limited, Cardiff, UK; ²Biotage, Charlotte, NC
- MP 784 **Assessing Efficiency of Matrix Cleanup using Concise LC-QQQ Methods of Lipid Detection;** Irina Dioumaeva¹; Bruce Richter²; ¹Agilent Technologies, Inc., Lake Forest, CA; ²Agilent technologies, Inc., Little Falls, DE
- MP 785 **Evaluation of Electrospray Ionization Effects on Jurkat-T Human Leukemia Cell Washing Buffers & Lipid Extraction Methods by LC-MS;** Candice Ulmer¹; Jing Chen²; Timothy Garrett³; Clayton Matthews²; Richard A. Yost¹; ¹Dept. of Chemistry, Univ of Florida, Gainesville, FL; ²Immunology & Laboratory Science, Univ of Florida, Gainesville, FL; ³CTSI, Dept. of Pathology, Univ of Florida, Gainesville, FL
- MP 786 **The Impact of Euthanasia Methods and Preanalytical Sample Handling in Lipid Analysis;** Fredrik Jernerén⁴; Jörg Hanrieder²; Marcus Söderquist³; Oskar Karlsson¹; ¹Uppsala University, Uppsala, Sweden; ²Chalmers Tech. University, Gothenburg, Sweden; ³Denator, Uppsala, Sweden; ⁴University of Oxford, Oxford, UK



7:30 – 8:00 am..... Set up all Tuesday posters
 10:30 am – 1:00 pm..... Odd-numbered posters present
 12:00 – 2:30 pm..... Even-numbered posters present
 7:30 – 8:00 pm..... Remove all Tuesday posters

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- TP 001 **High-Throughput Single Cell Profiling via Optically-Guided MALDI-TOF MS;** Ta-Hsuan Ong; David Kissick; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 002 **Imaging of Lipids in Kidney using Silver Nanoparticles;** Shelley N Jackson¹; Ajay Kailas¹; Ludovic Muller¹; Aurelie Roux¹; J Albert Schultz²; Amina S. Woods ¹; ¹*NIDA-IRP, NIH, Baltimore, MD*; ²*Ionwerks Inc, Houston, TX*
- TP 003 **Imaging of N-linked Glycans from Formalin-fixed Paraffin-embedded Tissue Sections Using MALDI Mass Spectrometry;** Shadi Toghi Eshghi; Shuang Yang; Punit Shah; Jered Pasay; Xingde Li; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
- TP 004 **Lipid Visualisation and Identification through collision Cross Section Aided Correlation of MALDI Imaging and MS/MS Fragmentation Data Sets;** Mark Towers; Emmanuelle Claude; Johannes Pc Viissers; *Waters Corporation, Manchester, UK*
- TP 005 **Comprehensive Characterization of the Mouse Brain Proteome Sampled in Mass Spectrometry Imaging studies;** Bram Heijis¹; Ricardo J. Carreira¹; Reinald Shyti²; Arn van den Maagdenberg²; Peter van Veelen³; Liam McDonnell¹; ¹*Center for Proteomics and Metabolomics, LUMC, Leiden, The Netherlands*; ²*Department of Human Genetics, LUMC, Leiden, The Netherlands*; ³*Dept of Immunohematology & Blood Transfusion, LUMC, Leiden, The Netherlands*
- TP 006 **Correlated Imaging Mass Spectrometry and Raman Spectroscopy for Oncology and Drug Resistance;** Dorothy Ahlf¹; Amanda B. Hummon²; Paul Bohn²; ¹*University of Notre Dame, South Bend, IN*; ²*University of Notre Dame, Notre Dame, IN*
- TP 007 **On-Chip Characterization of Brain Tumor Heterogeneity and Single-Cell Drug Susceptibility Analysis by Mass Spectrometry Imaging;** David Calligaris¹; Denis Loginov²; Revaz Machaidze¹; Isaiah Norton¹; Daniel R. Feldman³; John A. Alberta⁴; Charles D. Stiles⁴; Christopher J. Love²; Nathalie Y. R. Agar¹; ¹*Department of Neurosurgery, BWH/HMS, Boston, MA*; ²*Department of Chemical Engineering, MIT, Cambridge, MA*; ³*Department of Pathology, BWH/HMS, Boston, MA*; ⁴*Department of Cancer Biology, DFCI/HMS, Boston, MA*

- TP 008 **Improved Spatial Resolution in the Analysis of FFPE Tissue after Tryptic Digestion;** Janine Beckmann¹; Nannan Tao²; Janina Oetjen³; Detlev Suckau¹; Theodore Alexandrov⁴; Michael Becker¹; ¹*Bruker Daltonik GmbH, Bremen, GERMANY*; ²*Bruker Daltonics Inc., Fremont, CA*; ³*MALDI Imaging Lab, University of Bremen, Bremen, Germany*; ⁴*Center for Industrial Mathematics, Bremen, Germany*
- TP 009 **Assessment of Blood-Brain Barrier Crossing using MSI: New Predictive Tools for CNS Targeted Drug Efficacy Study;** Gregory Hamm; Fabien Pamelard; David Bonnel; Raphael Legouffe; Guillaume Hochart; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, FRANCE*
- TP 010 **3D Imaging of TiO₂ Nanoparticle Exposure Effects on Tetrahymena pyriformis;** Tina B. Angerer; John S. Fletcher; *University of Gothenburg, Gothenburg, Sweden*
- TP 011 **Toward Quantitative Infrared Matrix Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Mass Spectrometry Imaging of Biological Tissue;** Mark Bokhart¹; Guillaume Robichaud¹; Jeremy Barry¹; Angela Kashuba²; Craig Sykes²; David Muddiman¹; ¹*North Carolina State University, Raleigh, NC*; ²*The University of North Carolina, Chapel Hill, NC*
- TP 012 **Quantitative Laser Desorption Ionization Mass Spectrometry Imaging of Elements Directly in Histological Tissue Sections;** Jinrui Gan; Mohammadreza Shariatgorji; Anna Nilsson; Patrik Kallback; Per E. Andren; *Uppsala University, Uppsala, Sweden*
- TP 013 **On tissue Chemical Derivatization of Primary Amines: Application to Quantitative MALDI-MS Imaging of Neuropeptides and Amino Acids;** Mohammadreza Shariatgorji¹; Oskar Karlsson¹; Anna Nilsson¹; Henrik Lodén¹; Xiaoqun Zhang²; Per Svenningsson²; Per E. Andren¹; ¹*Uppsala University, Uppsala, Sweden*; ²*Karolinska Institutet, Stockholm, Sweden*

Imaging MS: Small Molecules and Drugs, 014 - 046

- TP 014 **Quercetin as a Highly Efficient MALDI Matrix for Negative-Ion Tissue Imaging by FTICR-MS;** Xiaodong Wang¹; Jun Han¹; Juncong Yang¹; Jingxi Pan¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; ²*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*

- TP 015 **Mass Spectrometry Imaging Data Co-Registered with Allen Brain Atlas Reveals the Accumulation of fatty Acids in the Hindbrain of MFP-2 Deficient Mice;** Karolina Škrášková^{1,2}; Gert Eijkel¹; Myriam Baes³; Paul P. Van Veldhoven⁴; Stephanie de Munter³; Artem Khmelinski^{5,6}; Walid M. Abdelmoula⁶; Jouke Dijkstra⁶; Ron M.A. Heeren^{1,2}; ¹FOM Institute AMOLF, Amsterdam, The Netherlands; ²TI-COAST, Amsterdam, The Netherlands; ³Laboratory of Cellular Metabolism, KU Leuven, Leuven, Belgium; ⁴LIPIT, KU Leuven, Leuven, Belgium; ⁵Percuro B.V., Enschede, The Netherlands; ⁶Department of Radiology, LUMC, Leiden, The Netherlands
- TP 016 **Quantitative Molecular Imaging of Neurotransmitters Measured Directly from Histological Tissue Sections in Experimental Models of Parkinson's Disease;** Mohammadreza Shariatgorji¹; Anna Nilsson¹; Nicoletta Schintu²; Richard J. A. Goodwin¹; Xiaoqun Zhang²; Alan Crossman³; Erwan Bezdard⁴; Per Svenningsson²; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institutet, Stockholm, Sweden; ³University of Manchester, Manchester, UK; ⁴University of Bordeaux 2, Bordeaux, France
- TP 017 **Detection of Ammonia on Human Colon Cancer-Bearing Livers of Superimmunodeficient NOG Mice by MALDI MS Imaging;** Akiko Kubo^{1,2}; Mitsuyo Ohmura¹; Tsuyoshi Nakanishi³; Makoto Suematsu^{1,2}; ¹Keio University, Tokyo, Japan; ²ERATO Suematsu gas biology project, Tokyo, Japan; ³Shimadzu Corporation, Kyoto, Japan
- TP 018 **Food-induced Changes of Lipids and Vitamins in Rat Neuronal and Intestinal Tissue Visualized by Imaging ToF-SIMS;** Masoumeh Dowlatshahpour²; Eva Jennische³; Stefan Lange³; Per Malmberg¹; Andrew Ewing¹; ¹University of Gothenburg, Gothenburg, Sweden; ²Chalmers University of Technology, Gothenburg, Sweden; ³Institute of Biomedicine, Gothenburg, Sweden
- TP 019 **Characterizing the Chemotypic Landscape of Polymicrobial Biofilms;** Vanessa Phelan¹; Julieta Aguilar¹; Kit Pogliano¹; Pieter Dorrestein²; ¹UC, San Diego, La Jolla, CA; ²University of California, San Diego, Skaggs school, La Jolla, CA
- TP 020 **High Resolution Mass Spectrometry Imaging of Plant Tissues: Towards a Plant Metabolome Atlas;** Andreas Roempp¹; Dhaka Bhandari¹; Wolfgang Friedt²; Sven Gottwald²; Bernhard Spengler¹; ¹Analytical Chemistry, Justus Liebig University, Giessen, Germany; ²Plant Breeding, Justus Liebig University, Giessen, Germany
- TP 021 **MALDI/LDI-FTICR Mass Spectrometry Imaging for Plant Tissue Analysis to Distinguish Changes in Metabolite Distributions under Different Stimulus Environments;** Katsutoshi Takahashi; *Nat'l Institute Advan. Indus. Sci Tech, Tokyo, Japan*
- TP 022 **Chemical Interface of Plant-Pathogen Interactions Explored by MALDI MS Imaging;** Adam Klein^{1,2}; Gargey Yagnik^{1,2}; Rebecca Hansen^{1,2}; Young Jin Lee^{1,2}; ¹Iowa State University, Ames, IA; ²Ames Laboratory-USDOE, Ames, IA
- TP 023 **Biopsy Analysis Using Flowprobe Mass Spectrometry;** Mariam S Elnaggar¹; Brendan Prideaux²; Veronique Dartois²; Justin Wiseman¹; ¹Prosolia, Inc., Indianapolis, IN; ²PHRI, Newark, NJ
- TP 024 **Investigating Absolute Quantitation of Small Molecule Drugs Profiled in Tissue Sections using Liquid Extraction Surface Analysis (LESA)-MRM analysis;** Edward Takach; Tom Clinckemaillie; Thomas O'Shea; Hanlan Liu; *Sanofi, Waltham, MA*
- TP 025 **ESI-MS Fingerprinting and HPTLC/DESI-MS Imaging of the Crude Extract from the Peels of *Citrus aurantium* L. (*Rutaceae*);** Bianca Bagatela^{1,2}; Andrey Lopes^{1,2}; Elaine Cristina Cabral¹; Fábio Perazzo²; Demian Ifa¹; ¹York University, Toronto, ON, Canada; ²UNIFESP, São Paulo, SP, Brazil
- TP 026 **Imaging and Spatial Profiling of Anti-Tuberculosis Drugs in Tissue using Liquid Microjunction Surface Extraction, MALDI-MS Imaging, and Micro-Dissection LC-MS/MS;** Brendan Prideaux¹; Mariam S Elnaggar²; Jansy Sarathy¹; Matthew Zimmerman¹; Justin Wiseman²; Veronique Dartois¹; ¹Public Health Research Institute, Rutgers, Newark, NJ; ²Prosolia, Inc., Indianapolis, IN
- TP 027 **High Sensitive Quantitation of Raclopride in Rat Brain by Liquid Extraction Surfaced Analysis Mass Spectrometry;** Jun Tadano; Toichiro Yamada; Kenichi Watanabe; Tetsuya Nakagawa; Masashi Yabuki; *Dainippon Sumitomo Pharma Co., Ltd., Suita, Japan*
- TP 028 **Drug Distribution and Pharmacokinetics in an Orthotopic Brain Tumor Model by MS Imaging and LCMS;** Stacey R. Oppenheimer¹; Matt Teague¹; Justine Lam²; Jinwei Wang²; Konstantinos Tsaparikos²; Hui Wang²; Justin Stroh¹; Emily Miller¹; Wei Song¹; Tod Smeal²; Ted W. Johnson²; ¹Pfizer, Groton, CT; ²Pfizer, La Jolla, CA
- TP 029 **A Nano-PALDI Approach for Absolute Quantitation of Anticancer Drugs in Tumor Tissues;** Enrico Davoli; Roberta Pastorelli; Massimo Zucchetti; Silvia Giordano; Lavinia Morosi; *IRCCS Istituto Mario Negri, Milano, Italy*
- TP 030 **Spatially Correlated Quantitative MALDI Analyses of Rifampicin in Liver;** Chad W. Chumbley¹; Michelle L. Reyzer¹; Gwendolyn A. Marriner²; Laura E. Via²; Clifton E. Barry, III²; Richard M. Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²NIAID, National Institutes of Health, Bethesda, MD
- TP 031 **Imaging LA-ICP-MS as a Powerful Tool for the Investigation of Toxic Mercury Species in *Drosophila melanogaster*;** Ann-Christin Niehoff¹; Stefanie Fingerhut²; Sabrina Kröger²; Oliver Bolle Bauer²; Jacqueline Schulz⁴; Sören Meyer¹; Michael Sperling²; Astrid Jeibmann⁴; Tanja Schwerdtle³; Uwe Karst²; ¹NRW Graduate School of Chemistry, Münster, Germany; ²Westfälische Wilhelms-Universität Münster, Münster, Germany; ³Universität Potsdam, Nuthetal, Germany; ⁴University Hospital Münster, Münster, Germany
- TP 032 **Quantitative LA-ICP-MS Imaging of Silver in Different Target Organs of Rats after Intratracheal Instillation of Silver Nanoparticles;** Franziska Blaske; Olga Reifschneider; Mandy Grossgarten; Michael Sperling; Uwe Karst; *Westfälische Wilhelms-Universität Münster, Muenster, GERMANY*
- TP 033 **Effects of Oral Administration of Methylphenidate on *Drosophila* Brain Studied by Imaging Mass Spectrometry;** Nhu Phan¹; Amir Mohammadi²; Masoumeh Pour²; Jörg Hanrieder²; John Fletcher¹; Andrew Ewing^{1,2}; ¹Gothenburg University, Gothenburg, Sweden; ²Chalmers University of Technology, Gothenburg, Sweden
- TP 034 **PET Ligand distribution in rat brain by MALDI Imaging: Impact of the tissue preparation on Raclopride distribution;** Emeline Falaux; David Bonnel; Gregory Hamm; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, France*
- TP 035 **Visualizing First Pass Hepatic Metabolism of Amodiaquine using MALDI Mass Spectrometry Imaging;** Stephanie Dale³; Beth DiTondo¹; Kerstin Strupat²; Patrick Rudewicz³; ¹AB SCIEX, Framingham, MA; ²Thermo Fisher Scientific, Bremen, Germany; ³Novartis, Emeryville, CA
- TP 036 **Identification of the Neuroanatomical Substrate Involved in ICVNPY Inhibitory Effects on Reinstatement of Cocaine-Induced Behavior in Rats by MALDI IMSite;** Leila Hosseinzadehshahri; *Student, Buffalo, NY*

- TP 037 **Visualization of Lipids and Small Metabolites in *Arabidopsis thaliana* Seed by MALDI-MS imaging;** Maria Dueñas^{1,2}; Andrew Korte^{1,2}; Kent Chapman³; Drew Sturtevant³; Young Jin Lee^{1,2}; ¹Iowa State University, Ames, IA; ²Ames Laboratory US Dept. of Energy, Ames, IA; ³University of North Texas, Denton, TX
- TP 038 **Mapping Regional Localization in Rat Brain of Reduced Lipoic Acid by Laser Ablation Electrospray Ionization Tandem Mass Spectrometry (LAESI-MS/MS);** Marina Galvez-Peralta¹; Callee M. Walsh²; Aric F. Logsdon¹; Jason D. Huber¹; Paul R. Lockman¹; Patrick S. Callery¹; ¹West Virginia University, Morgantown, WV; ²Protea Biosciences, Morgantown, WV
- TP 039 **Mapping Metabolite and Protein Changes in the Cataractous Lens using MALDI Imaging Mass Spectrometry;** Mitchell G. Nye-Wood¹; Jeffrey Spraggins²; Richard M. Caprioli²; Kevin L. Schey²; Paul J. Donaldson¹; Angus C. Grey¹; ¹University of Auckland, Auckland, New Zealand; ²Vanderbilt University, Nashville, TN
- TP 040 **High Spatial Resolution Laser Microdissection LC-MS/MS analysis of rat liver histology samples;** Paul Moench; Christopher DeBenedetto; James Glick; Robert Johnson; Jimmy Flarakos; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- TP 041 **A Multidimensional Approach for Identification of Isobaric Lipids Detected in Direct MS Analysis and Imaging of Human Liver;** Joscelyn Sarsby¹; Alan Race¹; Patricia F. Lalor¹; Josephine Bunch²; Helen Cooper¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, London, UK
- TP 042 **Strategies for Optimizing Detection of Endogenous Metabolites Directly from Tissue via MALDI MS;** Michelle L. Reyzer; Jeffrey Spraggins; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- TP 043 **Finding Biomarkers in *Arabidopsis* FERONIA Receptor Kinase using MALDI-MSI;** Rebecca Hansen^{1,2}; Gargey Yagnik^{1,2}; Young Jin Lee^{1,2}; ¹Iowa State University, Ames, IA; ²Ames Laboratory-USDOE, Ames, IA
- TP 044 **Phenotype Determination of *Caenorhabditis Elegans* with Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging;** Robert Menger; Chaevien Clendinen; Louis Searcy; Richard A. Yost; Arthur S. Edison; *University of Florida, Gainesville, FL*
- TP 045 **Characterizing the Novel Synthetic Cannabinoid, RCS-4's Metabolism – Human Hepatocytes Applicability in Clinical and Forensic Drug Testing;** Adarsh Gandhi¹; Mingshe Zhu²; Shaokun Pang³; Ariane Wohlfarth⁴; Karl Scheidweiler⁴; Marilyn Huestis⁴; ¹Lundbeck Research USA Inc., Paramus, NJ; ²Bristol-Myers Squibb, Princeton, NJ; ³AB SCIEX, San Diego, CA; ⁴NIDA, NIH, Baltimore, MD
- TP 046 **Classification of Drug Induced Toxicology in Tissue Samples using MALDI Mass Spectrometry Imaging;** Anna Nilsson¹; Richard Goodwin²; Benita Forngren³; Suzanne Iverson⁴; Johan Lindberg⁵; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²AstraZeneca, Macclesfield, UK; ³former AstraZeneca, Södertälje, Sweden; ⁴AstraZeneca, Göteborg, Sweden; ⁵Swedish Toxicology Sciences Research Center, Södertälje, Sweden
- Imaging MS: Disease Markers, 047 - 073**
- TP 047 **Quantitative 3D MALDI-MS Imaging of Neurotransmitters and Metabolites in Aging Models of the Mouse Brain;** Mohammadreza Shariatgorji¹; Anna Nilsson¹; Dennis Trede^{2,3}; Theodore Alexandrov^{2,4}; Nicoletta Schintu⁵; Per Svenningsson⁶; Per E. Andren¹; ¹Uppsala University, Uppsala, Sweden; ²SciLS GmbH, Bremen, Germany; ³Steinbeis Innovation Center SciLS Research, Bremen, Germany; ⁴University of Bremen, Bremen, Germany; ⁵Karolinska Institutet, Stockholm, Sweden
- TP 048 **Spatial Metabolites and Lipids Profiling in a Rat Model of Experimental Autoimmune Myocarditis by Matrix-assisted Laser Desorption/Ionization Imaging Mass Spectrometry;** Jin Woo Jung¹; Kwan Soo Hong²; Geum-Sook Hwang¹; Jungju Seo¹; ¹Korea Basic Science Institute, Seoul, South Korea; ²Korea Basic Science Institute, Ochang, South Korea
- TP 049 **Classification of Soft Tissue Sarcomas using MALDI Imaging Mass Spectrometry;** Sha Lou; Benjamin Balluff; Marieke A. de Graaf; Judith V.M.G. Bovée; Liam A. McDonnell; *Leiden University Medical Center, Leiden, the Netherlands*
- TP 050 **Importance of Tissue Suppression Effect on Biomarkers by MSI–Application to Mouse Xenografts;** Guillaume Hochart¹; Fred Fack²; David Bonnel¹; Olivier Keunen²; Simone P. Niclou²; Jonathan Stauber¹; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²Norlux Neuro-Oncology Laboratory, CRP-Santé, Luxembourg, Luxembourg
- TP 051 **Discrimination of Metastasis from Breast and Pancreatic Cancer by MALDI Imaging;** Rita Casadonte¹; Mark Kriegsmann³; Katrin Friedrich⁴; Gustavo Baretton⁴; Mike Otto^{1,2}; Soeren Deininger⁵; Detlev Suckau⁵; Martin Schuerenberg⁶; Jörg Kriegsmann^{1,2}; ¹Proteopath, Trier, Germany; ²Center for Histology, Cytology & Mol. Diagnostics, Trier, Germany; ³University of Heidelberg, Department of Pathology, Heidelberg, Germany; ⁴University of Dresden, Department of Pathology, Dresden, Germany; ⁵Bruker Daltonik GmbH, Bremen, Germany
- TP 052 **De Novo Discovery of Tumor Clones Linked to Metastasis and Poor Prognosis Using MALDI Imaging Mass Spectrometry;** Benjamin Balluff¹; Christian Frese⁴; Stefan Maier⁵; Cedrik Schoene²; Bernhard Kuster³; Manfred Schmitt⁶; Michaela Aubele²; Heinz Hoefler²; André Deelder¹; Albert Heck⁴; Johannes Morreau¹; A.F. Maarten Altelaa⁴; Axel Walch²; Liam McDonnell¹; ¹Leiden University Medical Center, Leiden, Netherlands; ²Helmoltz Zentrum Muenchen, Munich, Germany; ³Technical University Munich, Freising, Germany; ⁴Utrecht University, Utrecht, N/A; ⁵TU Muenchen, Freising, Germany; ⁶Klinikum Rechts der Isar, Munich, Germany
- TP 053 **Histodiagnostic Differentiation of Primary Mamma Carcinoma Tumor and Metastasis by MALDI-TOF Imaging and Intact Cell Mass Spectrometry;** Sophie Froehlich¹; Donscho Kerjaschki²; Guenter Allmaier¹; Martina Marchetti-Deschmann¹; ¹Vienna University of Technology, Vienna, Austria; ²Medical University Vienna, Vienna, Austria
- TP 054 **Validation of Mass Spectrometry Imaging as a Tool for the Detection of Cancer Tissue in Tissue Sections;** Olga Kraus¹; Pierre Abramowski²; Kristoffer Riecken²; Boris Fehse²; Sascha Rohn³; Hartmut Schlüter¹; ¹Clinical Chemistry, University Hamburg Eppendorf, Hamburg, Deutschland; ²Research Department Cell and Gene Therapy, Clinic, Hamburg, *uswählen (nur für USA / Kan. / Aus.)*; ³Institute of Food Chemistry, University Hamburg, Hamburg, *uswählen (nur für USA / Kan. / Aus.)*
- TP 055 **Identification and Spatial Localization of Proteins from Mouse Brain Tumor Using a Combination of MALDI Imaging and LC-MALDI;** Sergei Dikler¹; Daniel R. Feldman²; Jennifer L. Ide²; Mark A. Marchionni³; Charles D. Stiles³; Nathalie Y.R. Agar^{2,3}; ¹Bruker Daltonics, Billerica, MA; ²Brigham and Women's Hospital, HMS, Boston, MA; ³Dana-Farber Cancer Institute, HMS, Boston, MA
- TP 056 **Proteomic Analysis of Formalin-Fixed Paraffin-Embedded Renal Amyloidosis Tissues using MALDI Imaging Mass Spectrometry;** Rita Casadonte¹; Mark

- Kriegsmann²; Mike Otto^{1,3}; Rainer Paape⁴; Detlev Suckau⁴; Sören-Oliver Deininger⁴; Kerstin Amann⁵; Jörg Kriegsmann^{1,3}; ¹Proteopath GbR, Trier, Germany; ²University of Heidelberg, Department of Pathology, Heidelberg, Germany; ³Center for Histology, Cytology and Molecular Diagn, Trier, Germany; ⁴Brüker Daltonik GmbH, Bremen, Germany; ⁵University of Erlangen-Nuremberg, Erlangen, Germany
- TP 057 **Differences in the Proteomic Pattern of Colon and Pancreatic Carcinoma using High-Throughput Imaging Mass Spectrometry (IMS);** Jörg Kriegsmann^{1,5}; Mark Kriegsmann²; Vanessa Schommer¹; Daniela Aust³; Gustavo Baretton³; Sören-Oliver Deininger⁴; Detlev Suckau⁴; Mike Otto^{1,5}; Rita Casadonte⁵; ¹Center for Histology, Cytology and Molecular Diagn, Trier, Germany; ²University of Heidelberg, Department of Pathology, Heidelberg, Germany; ³University of Dresden, Department of Pathology, Dresden, Germany; ⁴Brüker Daltonik GmbH, Bremen, Germany; ⁵Proteopath GbR, Trier, Germany
- TP 058 **Imaging Mass Spectrometry to Uncover Proteomic Differences in Non-Hodgkin's Lymphomas;** Kristina Schwamborn¹; Martina Rudelius²; Richard Caprioli³; ¹Technical University Munich, Munich, Germany; ²University of Würzburg, Würzburg, Germany; ³Vanderbilt University, Nashville, TN
- TP 059 **Multimodal Imaging Mass Spectrometry for Probing the Protein-Lipid Interplay Underlying Amyloid-Beta Plaque Formation in Experimental Alzheimers Disease;** Jörg Hanrieder^{1,2}; Stina Syvänen³; Andrew G. Ewing^{1,2}; ¹Chalmers Tech. University, Gothenburg, Sweden; ²National Center for Imaging Mass Spectrometry, Gothenburg, Sweden; ³Uppsala University, Uppsala, Sweden
- TP 060 **MALDI Imaging of Lipid and Protein Changes in the Human Alzheimer's Disease Hippocampus;** Angus C. Grey; Lakshini Mendis; Richard L.M. Faull; Maurice A. Curtis; *Auckland University, Auckland, New Zealand*
- TP 061 **Tracking Cholesterol Distribution following Plaque Formation in a Mouse Model of Atherosclerosis using Dietary d6-cholesterol and MALDI Imaging Mass Spectrometry;** Nathan Hatcher¹; Jose Castro-Perez²; Vivienne Mendoza²; Nana Kofi Karikari¹; Karen Gagen²; Henry Shion³; Alan Millar³; John Shockcor³; David McLaren²; Vinit Shah²; Stephen Previs²; Karen Akinsanya²; Michele Cleary¹; Thomas P Roddy²; Douglas G Johns²; Sheng-Ping Wang²; ¹Merck Research Labs, West Point, PA; ²Merck Research Labs, Kenilworth, NJ; ³Waters Corporation, Milford, MA
- TP 062 **Mass Spectrometry Imaging of Breast Tumor Hypoxia Using 2-Nitroimidazoles as Chemical Markers;** Nadine E. Mascini¹; Asif Rizwan²; Lu Jiang²; Menglin Cheng²; Kristine Glunde²; Ron M.A. Heeren¹; ¹FOM Institute AMOLF, Amsterdam, Netherlands; ²Johns Hopkins University, Baltimore, MD
- TP 063 **Imaging MS Sheds Light on What's Happening in Traumatic Brain Injury;** Ludovic Muller^{1,2}; Aurelie Roux¹; Shelley N Jackson¹; Brian M Cox³; J Albert Schultz⁴; Amina S Woods¹; ¹NIH/NIDA-IRP, Baltimore, MD; ²University of Pittsburgh, Pittsburgh, PA; ³Uniformed Services University, Bethesda, MD; ⁴Ionwerks, Houston, TX
- TP 064 **Profiling and Imaging of Lipids in Demyelinated Rat Spinal Cord Using Mass Spectrometry;** Roberto Fernandez¹; Pau Gonzalez²; Javier Díez-García³; Begoña Castro³; Francisco J. Rodríguez²; Jose A. Fernandez¹; ¹Universidad del País Vasco, Leioa, Spain; ²Hospital Nacional de Paraplégicos, Toledo, Spain; ³Histocell S. L., Derio, Spain
- TP 065 **Defining the Tissue Distribution of Glycosphingolipid Species in Model Tissue Systems using High Resolution MALDI Imaging Mass Spectrometry;** E. Ellen Jones¹; Shaalee Dworski²; Mustafa Kamani³; Jeffrey Medin^{2,3}; Tamara Nowling⁴; James Norris¹; Richard Drake¹; ¹Department of Cell and Molecular Pharmacology, MUSC, Charleston, South Carolina; ²Institute of Medical Science University of Toronto, Ontario, Canada; ³University Health Network, University of Toronto, Ontario, Canada; ⁴Division of Rheumatology & Immunology, MUSC, Charleston, SC
- TP 066 **MALDI-IMS of Brain Tissue from a Mouse Model of Timothy Syndrome;** William Friesen; Brian Schultz; Sarbajit Banerjee; Troy Wood; *SUNY at Buffalo, Buffalo, NY*
- TP 067 **MALDI-MSI Lipidomic Investigation into the Delayed Effect of Acute Radiation Exposure: The Lung Syndrome and Efficacy of a Medical Countermeasure;** Claire L. Carter; Jace W. Jones; Isabel Jackson; Zeljko Vujaskovic; Stephanie Tabisz; Allison Gibbs; Jamie Haper; Kory Barrow; Ann M. Farese; Thomas J. MacVittie; Maureen A. Kane; *University of Maryland, Baltimore, MD*
- TP 068 **MALDI-IMS Profiling of N-Linked Glycans in FFPE Tissue Blocks and On-tissue Characterization of Glycan Structures;** Richard R Drake¹; Powers Thomas¹; Yuan Shao¹; Haab Brian²; Anand Mehta³; ¹Medical University of South Carolina, Charleston, SC; ²Van Andel Research Institute, Grand Rapids, MI; ³Drexel University, Doylestown, PA
- TP 069 **A MALDI-IMS Workflow for Assessment of Global Changes in N-linked Glycan Profiles in Tumor Tissue Microarrays;** Thomas Powers¹; Benjamin Neely¹; Yuan Shao¹; Raymond Lance²; Dean Troyer²; Anand Mehta³; Brian Haab⁴; Richard R Drake¹; ¹Medical University of South Carolina, Charleston, SC; ²Eastern Virginia Medical School, Norfolk, VA; ³Drexel University, Doylestown, PA; ⁴Van Andel Research Institute, Grand Rapids, MI
- TP 070 **High Spatial and Mass Resolution Imaging of Human Age Matched Healthy and Age Related Macular Degenerated Retinal Tissue;** David M. Anderson¹; Zsolt Ablonczy²; Jeffrey Spraggins¹; Yannis Koutalos²; Rosalie Crouch²; Anne Hanneken³; Richard Caprioli¹; Kevin Schey¹; ¹Vanderbilt University School of Medicine, Nashville, TN; ²Medical University of South Carolina, Charleston, SC; ³The Scripps Research Institute, La Jolla, CA
- TP 071 **Mass Spectrometric Imaging in Malaria Research;** Saleh Mahmud Khalil; Andreas Römpf; Jette Pretzel; Katja Becker; Bernhard Spengler; *Giessen, GERMANY*
- TP 072 **Lipidomic analysis of Nipah Virus Infection in a Mouse Model by MALDI-MS Imaging;** Alexander Shavkunov¹; Bjorn Nilsson¹; Tatyana Yun²; Terry Juelich²; Jennifer Smith²; Alexander Freiberg²; Carol Nilsson¹; ¹Department of Pharmacology and Toxicology, UTMB, Galveston, TX; ²Department of Pathology, UTMB, Galveston, TX
- TP 073 **Oxidative Damage During Staphylococcus aureus Infection Revealed by High Mass Resolution MALDI Protein Imaging;** Jessica L. Moore¹; Jeffrey Spraggins²; Neal D. Hammer³; Kristie Lindsey Rose¹; Eric P. Skaar³; Richard M. Caprioli¹; ¹Vanderbilt University MSRC, Nashville, TN; ²Vanderbilt University, Nashville, TN; ³Vanderbilt University Medical Center, Nashville, TN
- Informatics: Peptide Identification and Characterization, 074 - 091**
- TP 074 **Automated Parameter Setting for Protein Database Searches;** Wilfred Tang; Yong Joo Kil; Chris Becker; Marshall W. Bern; *Protein Metrics Inc., San Carlos, CA*
- TP 075 **MS Amanda Stand-Alone for Integration into Proteomic Workflows;** Viktoria Dorfer¹; Peter Pichler²; Thomas

- Stranzl²; Stephan Winkler¹; Karl Mechtler²; ¹University of Applied Sciences Upper Austria, Hagenberg, Austria; ²IMP Vienna, Austria
- TP 076 **Mixture Peptide Identifications with Proteomic Software from Complex Mixtures in Isolation Events from Hybrid and Tribrid Mass Spectrometers**; Leeann Higgins¹; Todd Markowski¹; Pratik Jagtap¹; Susan K. Van Riper²; ¹University of Minnesota, St. Paul, MN; ²University of Minnesota, Minneapolis, MN
- TP 077 **Identifying Novel Peptide Sequence Variants from High Throughput RNA-Seq Data Via Flexible Proteomic Database Generation using the Galaxy Framework**; James Johnson¹; Gloria Sheynkman²; Pratik Jagtap³; Michael Shortreed²; Getiria Onsongo¹; Lloyd Smith²; Tim Griffin³; ¹Minnesota Supercomputing Institute, Minneapolis, MN; ²University of Wisconsin, Madison, WI; ³University of Minnesota, Minneapolis, MN
- TP 078 **Towards a Novel Unprecedentedly Comprehensive Protein Identification Strategy, Mass Spectrometry and Ribosome Profiling: The Perfect Match**; Jeroen Crappé¹; Alexander Koch¹; Elvis Ndah^{1,2}; Sandra Steyaert¹; Daria Gawron^{1,2}; Ellen De Meester¹; Sarah De Keulenaer¹; Petra Van Damme^{1,2}; Gerben Menschaert¹; ¹Ghent University, Ghent, Belgium; ²VIB, Ghent, Belgium
- TP 079 **A Mutated Peptide Database for the Analysis of Aberrant Protein Sequences in Cancer**; Xu Yang; Iuliana Lazar; ¹Department of Biological Sciences, Virginia Tech, Blacksburg, VA
- TP 080 **Accurate FDR (False Discovery Rate) Estimation for Database Searching in Proteogenomics Studies**; Yoonsung Joh¹; Hyunwoo Kim¹; Kyubaek Hwang²; Heejin Park¹; Eunok Paek¹; ¹Hanyang University, Seoul, KOREA; ²Soongsil University, Seoul, KOREA
- TP 081 **Proteogenomic Approach to Cancer Cell Line Differentiation using Exome-Derived Variant Peptides: NCI-60 Panel Case Study**; Maria A. Karpova¹; Dmitry S. Karpov¹; Mark V. Ivanov²; Alexey L. Chernobrovkin^{1,3}; Mikhail A. Pyatnitsky¹; Andrey V. Lisitsa¹; Alexander I. Archakov¹; Mikhail V. Gorshkov²; Sergei A. Moshkovskii¹; ¹Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Karolinska Institutet, Stockholm, Sweden
- TP 082 **Assessing Depth of Proteome Coverage Required for Novel Peptide Detection in Breast Cancer using Patient Derived Xenograft Models**; Kelly Ruggles¹; Zuoqian Tang¹; Zuya Wang¹; Jennifer Teubl¹; Manor Askenazi²; Christopher Maher³; Song Cao³; Li Ding³; Michael McLellan³; Karl Clauser⁴; Philipp Mertins⁴; Robert Kitchens³; Charles Perou⁵; Steven Carr⁴; R. Reid Townsend³; Sherri Davies³; Matthew Ellis³; David Fenyo¹; ¹NYU Langone Medical Center, New York, NY; ²Biomedical Hosting LLC, Arlington, MA; ³Washington University, St. Louis, MO; ⁴Broad Institute of MIT and Harvard, Boston, MA; ⁵University of North Carolina, Chapel Hill, NC
- TP 083 **IC: A New Peptide Identification Tool for Both Data-Dependent and Data-Independent Acquisition**; Sangtae Kim¹; Ying Sonia Ting²; Alex Hu²; Richard D. Smith¹; William Stafford Noble²; Michael J. Maccoss²; Samuel H. Payne¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Washington, Seattle, WA
- TP 084 **Peptide-Centric Database Search Engines Applied to Data Independent Acquisition UDMS^E Data**; Pedro Navarro; Jennifer Hahlbrock; Jörg Kuharev; Ute Distler; Stefan Tenzer; ¹Institute for Immunology, Univ. Medical Center, Mainz, Germany
- TP 085 **Direct Non-Targeted Protein Identification from Data Independent Acquisition (DIA) Data Using Database Search**; Ignat Shilov¹; Sean L. Seymour¹; Christie Hunter¹; Stephen A Tate²; Gordana Ivosev¹; Ahmad Hosseingholizadeh²; ¹AB Sciex, Redwood City, CA; ²AB SCIEX, Concord, ON
- TP 086 **Optimized Spectral Library Generation for HRM/SWATH Acquisition as Implemented in Spectronaut**; Tejas Gandhi; Roland M. Bruderer; Magdalena Bober; Vito Zanotelli; Oliver M. Bernhardt; Oliver Rinner; Lukas Reiter; ¹BiognoSYS AG, Zurich, Switzerland
- TP 087 **MSPLIT-SWATH: a New Spectral Library Search Algorithm for Data Independent Acquisition of Complex Protein Mixtures**; Jian Wang¹; Monika Tucholska²; Jean Philippe Lambert²; Brett Larsen²; Stephen A Tate³; Anne-Claude Gingras²; Nuno Bandeira¹; ¹UCSD, La Jolla, CA; ²Lunenfeld-Tanenbaum Research Institute, Toronto, ON; ³AB SCIEX, Concord, ON
- TP 088 **The Generating Function Approach for Peptide Identification in Spectral Networks**; Adrian Guthals¹; Christina Boucher²; Nuno Bandeira^{1,3}; ¹Department of Computer Science, UCSD, La Jolla, CA; ²Department of Computer Science, CSU, Fort Collins, CO; ³Skaggs School of Pharmacy and Pharm. Sci., UCSD, La Jolla, CA
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- TP 090 **A Better Scoring Function for Top-Down Spectral Deconvolution**; Qiang Kou¹; Xiaowen Liu^{1,2}; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²Indiana University School of Medicine, Indianapolis, IN
- TP 091 **Top-down Proteomics with a Bottom-up Algorithm**; Marshall W. Bern¹; Yong J. Kil¹; Wilfred Tang¹; Chris Becker¹; Xuemei Han²; John R. Yates, III²; Kristie Rose³; Dhananjay Sakrikar³; Kevin L. Schey³; Richard Caprioli³; ¹Protein Metrics Inc., San Carlos, CA; ²The Scripps Research Institute, La Jolla, CA; ³Vanderbilt University, Nashville, TN
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- TP 093 **Data-Independent Mass Spectrometry for the Analysis of Red Blood Cell Protein Degradation and Aging**; Huisong Pak¹; Pierre Lescuyer³; Markus Muller²; Alexander Scherl¹; ¹University of Geneva, Geneva, Switzerland; ²SIB, Geneva, Switzerland; ³Geneva University Hospital, Geneva, Switzerland
- TP 094 **A Computational Framework for Mining MS1 Data for Post Translational Modifications**; Bruce D. Pascal; Graham M. West; Yelenis Mari; Patrick R. Griffin; ¹The Scripps Research Institute, Scripps Florida, Jupiter, FL
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- TP 097 **Correction of Errors in Tandem Mass Spectrum Extraction Enhances Phosphopeptide Identification;** Piliang Hao; Yan Ren; James Tam; Siu Kwan Sze; *Nanyang Technological University, Singapore, Singapore*
- TP 098 **Algorithm for Accurate Estimation of False Localization Rates in Phosphoproteomics;** Thomas Taus¹; Thomas Köcher¹; Etienne Beltzung²; Gerhard Dürmberger^{1,3}; Karl Mechtler¹; ¹IMP/IMBA, Vienna, Austria; ²MFPL, Vienna, Austria; ³GMI, Vienna, Austria
- TP 099 **Evaluation of Accessible Database Searching Engines for Accurate Identification of Histone Post-Translational Modifications;** Zuofei Yuan; Shu Lin; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- TP 100 **SAHA Treatment Reveals the Link between Histone Lysine Acetylation and Proteome in Non-small Cell Lung Cancer A549 Cells;** Quan Wu¹; Lejie Cao¹; Xiaojun Peng²; Tieming He²; Zhongyi Cheng²; ¹Central Laboratory, Affiliated Provincial Hospital, Hefei, CN; ²PTM Biolabs, Inc, Hangzhou, China
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- TP 105 **Multiple PTMs Play a Role in the Regulation of Platelets in Health and Disease;** Florian Beck¹; Fiorella Solari¹; Stefan Loroch¹; Saskia Venne¹; Marc Vaudel²; Lennart Martens³; Ulrich Walter⁴; Johan Heemskerk⁵; Albert Sickmann¹; René Zahedi¹; ¹Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; ²Department of Biomedicine, University of Bergen, Bergen, Norway; ³VIB Ghent University, Ghent, Belgium; ⁴Center for Thrombosis and Hemostasis CTH, Mainz, Germany; ⁵Cardiovascular Research Institute CARIM, Maastricht, The Netherlands
- TP 106 **Comprehensive Profiling of Lysine Acetylome in Staphylococcus aureus;** Yi Zhang¹; Zhixiang Wu¹; Xuelian Wan¹; Ping Liu¹; Yingming Zhao²; Minjia Tan¹; ¹Shanghai Institute of Materia Medica, Shanghai, CHINA; ²the University of Chicago, Chicago, IL
- TP 107 **Variability in the Glycosylation Patterns of gp120 proteins from Different Human Immunodeficiency Virus Type 1 Isolates Expressed in Different Cells;** Ehwang Song¹; Samantha Rice-Williams²; Fan Jiang²; Ghalib Alkhatib²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²Southern Research Institute, Birmingham, AL
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- TP 109 **Automated Immunoaffinity-Based Proteomic Methods for the Study of Post-Translational Modification;** Matthew P. Stokes¹; Jeffrey C. Silva¹; Steven Murphy²; Jason Russell²; Jian Min Ren¹; Kimberly Lee¹; ¹Cell Signaling Technology, Danvers, MA; ²Agilent Technologies, Inc., Santa Clara, CA
- TP 110 **Protein and Glycoprotein LC/MS Using HILIC;** Barry Boyes^{1,2}; Ron Orlando²; Stephanie Schuster¹; Joseph Destefano¹; ¹Advanced Materials Technology Inc., Wilmington, DE; ²University of Georgia, Athens, GA
- TP 111 **A Phosphoproteomic Approach to Enrich and Identify Mono- and poly(ADP-ribosylation) Sites in Whole Cell Lysate;** Casey M. Daniels¹; Shao-En Ong²; Anthony K.L. Leung¹; ¹Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; ²University of Washington, Seattle, WA
- TP 112 **The Novel Lysine Glutarylation Pathway, Its Regulatory Enzyme SIRT5, Its Substrates and Regulatory Role in Metabolism;** Minjia Tan¹; Chao Peng²; Kristin A. Anderson³; Peter Chhoy³; Zhongyu Xie²; Lunzhi Dai²; Yi Zhang¹; Matthew D. Hirschey³; Yingming Zhao²; ¹Shanghai Institute of Materia Medica, Shanghai, CHINA; ²the University of Chicago, Chicago, IL; ³Duke University Medical Center, Durham, NC
- TP 113 **Site-Specific Quantitation of Lysine Acetylation in Isomeric Peptides of Histones H3 and H4;** Nebiyu Abshiru^{1,2}; Olivier Caron-Lizotte^{1,2}; Roshan Elizabeth^{1,2}; Alain Verreault^{1,2}; Pierre Thibault^{1,2}; ¹University de Montreal, Montreal, Canada; ²Institute for Research in Immunology and Cancer, Montreal, QC
- TP 114 **Affinity-based Quantitative Proteomics Reveals Non-histone Substrates of Methyltransferases G9a/GLP in Human Breast Adenocarcinoma Cell MDA-MB-231;** Xing-Jun Cao; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
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- TP 117 **Simultaneous Monitoring of Protein Methylation and Acetylation Expands the Post-Translational Modification Network in a Human Gastric Cancer Cell Line;** Hongbo Gu; Charles L. Farnsworth; Kimberly A. Lee; Jianmin Ren; Xiaoying Jia; Jeffrey C. Silva; *Cell Signaling Technology, Danvers, MA*
- TP 118 **PTM Directed Re-Wiring and Their Networks in Oncogene Mutant and Knock-Out Cancer Cells;** Jing Song; Benlian Wang; Zhenghe Wang; Mark R. Chance; *Case Western Reserve University, Cleveland, OH*
- TP 119 **Glycan Site Mapping of Glycoproteins in Serum;** Qiuting Hong; Evan Parker; Ting Song; Carlito Lebrilla; *Chemistry, UC, Davis, Davis, CA*
- TP 120 **Comprehensive Mapping of Ribosomal Protein Post-Translational Modifications by LC-MS/MS Analysis of Tryptic and Microwave-Assisted HCL Partial Hydrolysates;** Yuwei Chang; Rueyhung Weng; Chen-Chung Liao; Wailap Ng; *National Yang Ming University, Taipei, Taiwan*

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- TP 122 **Lysine Acetylome in *Streptomyces roseosporus* Reveals the Roles of Lysine Acetylation in Regulating Biosynthesis of Secondary Metabolites;** Guojian Liao¹; Xiaojun Peng²; Zhongyi Cheng²; Jianping Xie¹; ¹*College of Pharmaceutical Sciences, Southwest Univ, Chongqing, CN*; ²*PTM Biolabs, Inc, Hangzhou, China*
- TP 123 **Quantification of Lysine Acetylation in Human Oligodendroglia Cells in Response to Borna Disease Virus Infection;** Xia Liu^{1,2}; Xiaojun Peng³; Zhongyi Cheng³; Peng Xie^{1,2}; ¹*Institute of Neuroscience, Chongqing Medical Univ, Chongqing, CN*; ²*The First Affiliated Hospital, Chongqing Medical U, Chongqing, CN*; ³*PTM Biolabs, Inc, Hangzhou, China*
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- TP 125 **Elucidation of Diverse and Divergent Post-Translational Modification of Proteins in Closely Related Bacteria in a Natural Microbial Community without Enrichment;** Zhou Li^{1,2}; Yingfeng Wang²; Qiuming Yao³; Nicholas Justice⁴; Tae-Hyuk Ahn²; Dong Xu³; Robert Hettich^{1,2}; Jillian Banfield⁴; Chongle Pan^{1,2}; ¹*University of Tennessee, Knoxville, TN*; ²*Oak Ridge National Lab, Oak Ridge, TN*; ³*University of Missouri, Columbia, MO*; ⁴*University of California, Berkeley, CA*
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- TP 127 **Uncovering Novel Redox Regulated Cysteines in the Mitochondrial Proteome Governed by Distinct Sites of Reactive Oxygen Species Production;** Casey Quinlan¹; Bradford Gibson²; Martin Brand²; Jason Held³; ¹*Pfizer, La Jolla, CA*; ²*Buck Institute for Research on Aging, Novato, CA*; ³*Washington University Medical School, St. Louis, MO*
- TP 128 **Phosphorylation Dynamics of PTH Receptor Signaling in Osteoblasts;** Grace Williams; Jennifer Bethard; Mary Berkaw; Louis Luttrell; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- TP 129 **Isomer Proteomics: A Case Study of Epimerization and Isomerization in Crystallins;** Yuanqi Tao; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- TP 130 **Probing the Regulation of Ubc9 Activity using a Mass Spectrometry-Based *in vitro* SUMOylation Assay;** Francis McManus¹; Danielle Caron²; Frederic Lamoliatte¹; Pierre Thibault¹; ¹*Université de Montréal, Montréal, Canada*; ²*Université Laval, Québec, Canada*
- TP 131 **Evaluating the Relationship between N-glycosylation and Protein Stability in the Enteric Pathogen *Campylobacter jejuni*;** Joel Cain¹; Nichollas Scott²; Nestor Solis¹; Melanie White¹; Stuart Cordwell¹; ¹*The University of Sydney, Sydney, Australia*; ²*University of British Columbia, Vancouver, BC*
- TP 132 **Robust and Sensitive Methodologies of Chemical Crosslinking and Mass Spectrometry for Hybrid Structural Characterization of Endogenous Protein Complexes;** Yi Shi¹; Javier Fernandez-Martinez¹; Riccardo Pellarin²; Peter Fridy¹; Elina Tjioe²; Seung Joong Kim²; Qingjun Wang³; Andrej Sali²; Michael P. Rout¹; Brian T. Chait¹; ¹*The Rockefeller University, New York, NY*; ²*University of California, San Francisco, CA*; ³*University of Kentucky, Lexington, KY*
- TP 133 **Analysis of Ferritin and Apoferritin by MALDI-TOF with STJ Cryodetection;** Logan Plath¹; Alexander Aksenov²; Abdil Ozdemir³; David Sipe¹; Mark E. Bier¹; ¹*Carnegie Mellon University, Pittsburgh, PA*; ²*University of California - Davis, Davis, CA*; ³*Sakarya University, Adapazari, Turkey*
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- TP 136 **Optimizing an Orbitrap Mass Spectrometer for the High Resolution Analysis of Intact Mega Dalton Virus Capsids;** Joost Snijder¹; Michiel van den Waterbeemd¹; Eugen Damoc²; Eduard Denisov²; Dmitry Grinfeld²; Alexander Makarov^{1,2}; Albert J.R. Heck¹; ¹*Utrecht University, Utrecht, The Netherlands*; ²*Thermo Fisher Scientific, Bremen, Germany*
- TP 137 **The Monitoring of the Protein Complex Landscape in Response on Apoptosis using PCP-SILAC;** Nicholas Scott; Anders Kristensen; Leonard Foster; *University of British Columbia, Vancouver, Canada*
- TP 138 **Scoring Protein Interactions Using the CRAPome: A Contaminant Repository for Affinity Purification Mass Spectrometry Data;** Dattatreya Mellacheruvu¹; Zachary Wright¹; Anne-Claude Gingras²; Alexey Nesvizhskii¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON*
- TP 139 **Identification of Protein Interaction Partners of Protein Phosphatase 2A Catalytic Subunit Using Quantitative Mass Spectrometry;** Divyasri Damacharla¹; Xiangmin Zhang¹; Danjun Ma¹; Monique Lewis¹; Michael Caruso¹; Wissam Anteer¹; Yue Qi¹; Zhao Yang¹; Rodney Berry¹; Abdullah Mallisho¹; Zaher Msallaty¹; Sorin Draghici¹; Jeffrey Horowitz²; Berhane Seyoum¹; Zhengping Yi¹; ¹*Wayne State University, Detroit, MI*; ²*University of Michigan, Ann Arbor, MI*
- TP 140 **Identification of BK Protein Partners in Mouse Cerebellum using Proteomic Mass Spectrometry;** Lancia Darville; Bernd Sokolowski; *University of South Florida, Tampa, FL*
- TP 141 **New Interactors of the Peroxisomal Receptor Export Complex Revealed by Affinity Purification and SILAC Mass Spectrometry;** Jason Tonillo¹; Sascha Steltgens¹; Claudia Lindemann¹; Thilo Lerari¹; Helmut E. Meyer¹; Ralf Erdmann²; Katja Kuhlmann¹; ¹*Medical Proteome Center, Ruhr-University, Bochum, Germany*; ²*Institute of Physiol. Chemistry, Ruhr-University, Bochum, Germany*
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- TP 143 **Protein Phosphatase 1 Catalytic Subunit Protein Interaction Partners in Human Skeletal Muscle Revealed by Targeted Proteomics**; [Zhao Yang](#); Michael Caruso; Danjun Ma; Abdullah Mallisho; Berhane Seyoum; Monique Lewis; Xiangmin Zhang; Wissam Al-Janabi; Yue Qi; Divyarsi Damacharla; Rodney Berry; Zaher Msallaty; Sorin Draghici; Assia Shisheva; Zhengping Yi; *Wayne State University, Detroit, MI*
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- TP 212 **Rapid Detection of Bacterial Resistance by MALDI-TOF MS in Combination with Stable Isotope Labeling;** Jette Jung³; Sören Schubert³; Gary Kruppa²; Katrin Sparbier¹; Christoph Lange¹; Markus Kostrzewa¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA; ³Max-von-Pettenkofer Institute, Munich, Germany
- TP 213 **Sequence Level and Dual-phase Flagella Antigen Identification of Salmonella by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Keding Cheng; Angela Sloan; Julie Meakin; Stuart McCorrister; Morganne Jerome; Garrett Westmacott; Mike Drebot; Celine Nadon; J. David Knox; Gehua Wang; *Public Health Agency of Canada, Winnipeg, Canada*
- TP 214 **Study of MALDI Sample Preparation for Bacterial Identification;** Eun-kyeong Choi¹; Hanyoung Jung¹; Kyu Hwan Park¹; Yangsun Kim²; ¹Applied Surface Technology Inc., Suwon, KOREA; ²Hudson Surface Technology Inc., Old Tappan, NJ
- TP 215 **Recycling Old Software – Microbe Identification Using REIMS and MicrobeLynx;** Nicole Strittmatter²; Steven Pringle^{1,2}; Keith Richardson¹; Julia Balog^{2,3}; Laurence Firth¹; Zoltan Takats²; Lidia Cammack²; Mike Morris^{1,2}; ¹Waters Corporation, Manchester, UK; ²Imperial College London, London, UK; ³Medimass Ltd, Budapest
- TP 216 **MALDI-TOF MS Detection of Carbapenem Resistant Enterobacteriaceae and Pseudomonas aeruginosa;** Patrick Chong¹; Stuart McCorrister¹; Mark Unger²; David Boyd¹; Michael Mulvey¹; Garrett R Westmacott¹; ¹Public Health Agency of Canada, Winnipeg, Canada; ²University of Manitoba, Winnipeg, Canada
- TP 217 **Serovar and Strain Level Bacterial Differentiation Capabilities for 36 Closely Related Outbreak Strains by Intact Protein LCMS;** Melinda McFarland; Denis Andrzejewski; Peter Evans; John Callahan; *US Food & Drug Administration, College Park, MD*
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- TP 220 **A Rapid Fungal De-Replication/Identification Method Based on Laser Ablation Electrospray Ionization (LAESI) Mass Spectrometry Technology and Principle Component Analysis (PCA);** Lin Du¹; Haddon Goodman²; Robert Cichewicz¹; ¹University of Oklahoma, Norman, OK; ²Protea Biosciences, Inc., Morgantown, WV
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- TP 222 **An LC-MALDI Method for the Discovery and Identification of Markers of Antibiotic Resistance in Enterobacteriaceae;** Philippa Hart¹; Emmanuel Wey²; Timothy McHugh³; Indran Balakrishnan²; Omar Belgacem¹; ¹Shimadzu, Manchester, UK; ²Royal Free Hospital NHS Foundation Trust, London, UK; ³UCL Centre for Clinical Microbiology, London, UK
- TP 223 **The Structural Analysis of Oocyst Walls of Cryptosporidium, Toxoplasma, and Eimeria with Mass Spectrometry and Microscopy;** Edwin M. Motari¹; G. Guy Bushkin²; Jitender P. Dubey³; Catherine E. Costello⁴; Phillips W. Robbins¹; John Samuelson¹; ¹Boston University School of Dental Medicine, Boston, MA; ²Massachusetts Institute of Technology, Cambridge, MA; ³Animal Parasitic Diseases Laboratory, United State, Beltsville, MD; ⁴Boston University School of Medicine, Boston, MA
- TP 224 **Development of an LC-HRMS-based Metabolomic Approach to Study Methicillin-Resistant Staphylococcus aureus;** Sandrine Aros-Calt^{1,2}; Bruno Muller²; Céline Ducruix^{1,2}; Samia Boudah^{1,3}; Guillaume L'hostis²; Gaspard Gervasi²; Christophe Junot¹; François Fenaille¹; ¹LEMM-CEA-Saclay, Gif sur Yvette, France; ²bioMérieux, Marcy l'Etoile, France; ³GlaxoSmithKline - Centre de recherche F.Hyafil, Villebon-sur-Yvette, France
- TP 225 **Identification and Characterization of Francisella Strains by MALDI-TOF Detection for Biodefense Purposes;** Emie Durighello¹; Alain Lorphelin¹; Marie-Anne Roncato²; Eric Ezan³; Laurent Bellanger²; Jean Armengaud¹; ¹CEA, DSV/IBEB/SBTN/LBSP, Bagnols Sur Cèze, France; ²CEA, DSV/IBEB/SBTN/LICB, Bagnols sur Cèze, France; ³CEA, DSV/IBEB/SBTN, Bagnols sur Cèze, France
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- TP 228 **A Multi-Instrumental Targeted Proteomics Approach is Sufficient and Necessary for Comprehensive Analysis of Mycobacterial Protein Secretion;** Matthew M Champion; Emily Williams; George Kennedy; Patricia Digioseppe-Champion; *University of Notre Dame, Notre Dame, IN*
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- TP 231 **Cyanobacterial Agar-Based MALDI Mass Spectrometry Imaging;** Humberto Milagre¹; Beatriz Sandonato¹; Vanessa Santos²; Marcos Eberlin²; ¹UNESP, Araraquara, BRAZIL; ²UNICAMP, Campinas, Brazil

- TP 232 **Liquid Extraction Surface Analysis Mass Spectrometry of Intact Proteins from Bacterial Colonies;** Elizabeth C. Randall¹; Josephine Bunch²; Iain B. Styles¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, London, UK
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- TP 234 **Characterization of Antibody Drug Conjugates Prepared on Magnetic Protein A and G Particles by MS Analysis following IdeS Digestion;** Chris Hosfield¹; Becky Godat¹; Nidhi Nath¹; Archer Smith²; Philip Compton²; Paul Thomas²; Neil L. Kelleher²; Michael Rosenblatt¹; Marjeta Urh¹; ¹Promega, Madison, WI; ²Northwestern University, Evanston, IL
- TP 235 **Evaluation of an LC/MS Microfluidic Platform for Quantification of Intact Monoclonal Antibodies;** Catalin Doneanu; Brad Williams; Paul Rainville; Weibin Chen; Waters Corporation, Milford, MA
- TP 236 **Development of Integrated Informatics Workflows for the Automated Assessment of Comparability for Antibody Drug Conjugates (ADCs) using LC/UV and LC/UV/MS;** Robert Birdsall¹; Henry Shion¹; Frank Kotch²; April Xu³; Thomas Porter⁴; Weibin Chen¹; ¹Waters Corporation, Milford, MA; ²Pfizer Bioprocess Research & Development, Pearl River, NY; ³Pfizer Analytical Research & Development, Pearl River, NY; ⁴Pfizer Analytical Research & Development, Andover, MA
- TP 237 **Analysis of C1q Binding by Engineered IgG hexamers and the Initiation of Fluid Phase Complement Activation;** Guanbo Wang^{1,2}; Sara Rosati^{1,2}; Ewald T. J. van den Bremer³; Frank J. Beurskens³; Janine Schuurman³; Paul W.H.I. Parren³; Rob N. de Jong³; Albert J.R. Heck^{1,2}; ¹Utrecht University, Utrecht, The Netherlands; ²Netherlands Proteomics Center, Utrecht, The Netherlands; ³Genmab, Utrecht, The Netherlands
- TP 238 **The Characterization of Pentameric IgM (MORAb-028) using Enzymatic Digestion and LC-MS/MS: Disulfide Bond Assignment and Glycosylation Site Analysis;** Xin Cheng; Sara Jacob; Andrew Milinichik; Howard Turchin; Young Park; Wolfgang Ebel; Matthew Reeser; Luigi Grasso; Earl Albone; Morphotek Inc., Exton, PA
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- TP 240 **Conformational Difference in IgG2 Disulfide Isoforms Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry;** Zhongqi Zhang; Aming Zhang; Jing Fang; Robert Chou; Pavel Bondarenko; Amgen, Inc., Thousand Oaks, CA
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- TP 245 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody;** Ming Zhang^{1,2}; Bo An^{1,2}; Eslam Nouri-Nigjeh^{1,2}; Haoying Yu^{1,2}; Samuel Wopperer²; Jun Qu^{1,2}; ¹SUNY at Buffalo, Buffalo, NY; ²New York State Center of Excellence, Buffalo, NY
- TP 246 **High Sensitivity Native Antibody Drug Conjugate (ADC) Analysis using LC Mass Spectrometry;** Caroline S. Chu; Andy Gieschen; Ning Tang; Agilent Technologies, Santa Clara, CA
- TP 247 **Monoclonal Antibodies Complete Primary Structure and Biosimilarity Assessment in a Single Analysis using Transient Isotachopheresis Sheathless Capillary Electrophoresis-Tandem Mass Spectrometry;** Rabah Gahoual¹; Jean-Marc Busnel²; Johana Chicher³; Lauriane Kuhn³; Philippe Hamman³; Alain Beck⁴; Yannis Francois¹; Emmanuelle Leize-Wagner¹; ¹LSMIS, UMR-CNRS 7140, University of Strasbourg, Strasbourg, FRANCE; ²Beckman Coulter, Brea, CA; ³Institut de Biologie Moléculaire et Cellulaire, Strasbourg, France; ⁴Centre d'immunologie Pierre Fabre, Saint-Julien en Genevois, France
- TP 248 **Accurate Quantitation of Deamidated Peptides to Accelerate Formulation Process Development in Therapeutic Proteins;** Michael Peddicord¹; Difei Qiu¹; Ming Gu²; Yongdong Wang²; ¹Bristol-Myers Squibb, New Brunswick, NJ; ²Cerno Bioscience, Norwalk, CT
- TP 249 **Mass Spectrometry Imaging of Therapeutic Antibodies: Distribution of Trastuzumab in CB.17 SCID mice Implanted with the Human Breast BT474 Xenograft;** Aurore Tomezyk¹; David Bonnel¹; Chassidy Hall²; Robert J. Mullin²; Gregory Hamm¹; Kathryn Simon²; Jonathan Stauber¹; ¹ImaBiotech, MS Imaging Dept., Loos, France; ²Charles River Discovery Research Services, Morrisville, NC
- TP 250 **Disulfide Bond Analysis on Q Exactive Mass Spectrometry;** Xiaoxi Zhang¹; Jing Feng²; ¹ThermoFisher Scientific, Shanghai, China; ²Kawin Technology, Beijing, China
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- TP 255 **Comprehensive Structural Characterization of Biopharmaceuticals by Top-Down Mass Spectrometry and Hydrogen/Deuterium Exchange: Implications for Biosimilars;** Jingxi Pan¹; [Derek Smith](#)¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; ²*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*
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- TP 257 **Rapid and Structure-Specific LC/MS/MS Screening for Bioactive Glycan Motifs in Therapeutic Glycoproteins;** [Myung Jin Oh](#)¹; Serenus Hua¹; Youngsook Seo¹; Jong Shin Yoo²; Rudolf Grimm³; Hyun Joo An¹; ¹*AGRS, Chungnam National University, Daejeon, Korea*; ²*Korea Basic Science Institute, Ochang, Korea*; ³*Agilent Technologies, Santa Clara, CA*
- TP 258 **Characterization of Glycoengineered Biopharmaceuticals;** [Andres Guerrero](#)¹; Yanhong Li¹; Salem Alkanaimsh²; Lucas Arzola²; Bryce Hashimoto²; Minsook Hwang³; Aye Tu⁴; My Phu⁴; Abhaya Dandekar⁴; Bryce Falk³; Somen Nandi⁵; Raymond Rodriguez²; Karen McDonald²; Xi Chen¹; Carlito Lebrilla¹; ¹*UC Davis, Chemistry Department, Davis, CA*; ²*UC Davis, Chemical Engineering & Materials Science, Davis, CA*; ³*UC Davis, Plant Pathology, Davis, CA*; ⁴*UC Davis, Plant Science, Davis, CA*; ⁵*UC Davis, Molecular & Cellular Biology, Davis, CA*
- TP 259 **Rapid and Complete Structural Assignments of Recombinant Monoclonal Antibody Glycans;** [Ting Song](#); Sureyya Ozcan; Alicia Becker; Carlito Lebrilla; *University of California Davis, Davis, California*
- TP 260 **Biosimilar Glyco-analysis Comparison via Procainamide Labeling and Tandem LC-MS;** [Charles Nwosu](#); Natalie Yau; Steven Becht; *Pharmaceutical Product Development, Middleton, WI*
- TP 261 **2D UPLC and Synapt G2 Mass Spectrometry Facilitates mAb Biosimilar Study;** [Suping Zheng](#); Shirley Lin; Steve Becht; *PPD, Inc., Middleton, WI*
- TP 262 **Analysis of Monoclonal Antibody using High Flow HPLC coupled to Time-of-Flight Mass Spectrometry;** [Ravindra Gudihal](#)¹; Suresh Babu CV¹; Ning Tang²; ¹*Agilent Technologies India Pvt. Ltd, Bangalore, INDIA*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- TP 263 **Modular Workflow for Biosimilar Antibody Characterization at the Intact and Middle-Down Level;** [Zsolt Gengeliczki](#); Marcell Olajos; Tamás Kiss; János Varga; Krisztián Lenkey; Katalin Baranyáné Ganzler; *Gedeon Richter Plc., Budapest, Hungary*
- TP 264 **Structure Characterization and Differentiation of Biosimilar and Reference Products using Unique Combination of Complementary Fragmentation Mechanisms;** [Zhiqi Hao](#)¹; Fan Zhang²; Shiao-Lin Wu^{2,3}; David Horn¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*BioAnalytix, Cambridge, MA*; ³*Barnett Institute, Northeastern University, Boston, MA*
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- TP 266 **Absolute Quantification Strategies for Total Protein and Monosaccharide Concentration in a Monoclonal Antibody (IgG) using 'bottom-Up' ID LC-MS/MS Hydrolysis Techniques;** [Mark Lowenthal](#); Eric Kilpatrick; John Schiel; Karen Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
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- TP 268 **Determination of the Mycotoxin T2 from Oats by Direct Analysis in Real Time - Mass Spectrometry (DART-MS);** Mark Busman; *USDA, ARS, NCAUR, BFP, Peoria, IL*
- TP 269 **Profiling Beer: Solid Phase Micro-Extraction (SPME) Analysis via Direct Analysis in Real Time HRMS;** [Joseph Lapointe](#); Brian Musselman; Robert Goguen; *IonSense Inc., Saugus, MA*
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- TP 272 **Simultaneous Positive/Negative Dielectric Barrier Discharge Microplasma Ionization for Multiclass Organic Contaminants' Determination in complex matrices by LC/HRMS;** [Heiko Haven](#)^{1,2}; Bienvenida Gilbert-López³; Juan F Garcia-Reyes³; Antonio Molina-Díaz³; Joachim Franzke⁴; ¹*University of Wuppertal, Wuppertal, Germany*; ²*University of Muenster, Muenster, Germany*; ³*University of Jaén, Jaén, Spain*; ⁴*Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
- TP 273 **Analyses of Chlorinated Contaminants in Food Products by Atmospheric-Pressure Dissociative Electron Attachment Ionization;** Carina Minardi¹; Paolo Lecchi²; [Kaveh Jorabchi](#)¹; ¹*Georgetown Univ., Washington, DC*; ²*DSM Nutritional Products, Columbia, MD*
- TP 274 **Development and Validation of a Highly Sensitive LC-MS/MS Method for Quantitation and Confirmation of Oxytocin in Milk;** [Prasanth Joseph](#)¹; Praveen Kumar Sharma¹; Manoj Pillai¹; Sanjivan Bahman²; Ajit Dua²; S.S. Marwaha²; ¹*AB SCIEX, Gurgaon, INDIA*; ²*Punjab Biotechnology Incubator, Mohali, India*
- TP 275 **High Sensitivity Quantitation Method of Dicyandiamide and Melamine in Milk Powders by Liquid Chromatography Tandem Mass Spectrometry;** [Zhi Wei Ting](#)¹; Jing Cheng Ng²; Jie Xing¹; Zhaoqi Zhan¹; ¹*Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore Science Park 1, Singapore*; ²*Department of Chemistry, National University of Singapore, Singapore*; ^{*}*Student*
- TP 276 **Accurate Mass Screening of Nitrogenous Economic Adulterants in Milk Proteins;** Nicholas Cellar¹; Jonathan Draher¹; Nicholas Baldauf²; [Todime Reddy](#)¹; ¹*Abbott Laboratories, Columbus, OH*; ²*Advanced Testing Laboratory, Blue Ash, OH*
- TP 277 **Determination of Emerging Nitrogenous Economic Adulterants in Milk Proteins by HPLC/Compact Mass Spectrometry;** Stefan Ehling¹; Jonathan Draher¹; Nick Cellar¹; Todime Reddy¹; [Jack Henion](#)²; Nigel Sousou²; ¹*Abbott Nutrition, Columbus, OH*; ²*Advion, Inc., Ithaca, NY*
- TP 278 **Enhanced Reduction of Matrix Effects using LC-MS/MS with Online Extraction for the Rapid Quantitation of Antibiotics in Milk;** [Louis Maljers](#); Helen Qingyu Sun; *Bruker Daltonics Inc, Fremont, Ca*

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- TP 281 **Determination of Benzimidazole Residues in Animal Tissue by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry;** Yin Huo; Changku Li; Qian Sun; Jinting Yao; Song Zhan; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Guangzhou, CHINA*
- TP 282 **Rapid Determination of Residues of Beta-Agonists in Animal Tissues using Liquid Chromatography-Tandem Mass Spectrometry including Mass Spectral Library Searching;** Simon Ashton¹; David Baker¹; Neil Loftus¹; Simon Hird²; ¹*Shimadzu, Manchester, UK*; ²*The Food and Environment Agency, York, UK*
- TP 283 **Detection the Residues of Tetracycline Antibiotics in Pork and Chicken Meat by SPE-LC/MS/MS;** Xuan Su¹; Guotao Lu²; ¹*Bonna Agela Technologies. Ltd, Tianjin, China*; ²*Bonna Agela Technologies. Inc, Wilmington, DE*
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- TP 285 **Quantitative Analysis of Anabolic Steroids in Control Samples from Food-Producing Animals using a Column-Switching LC-HESI-MS/MS Assay;** John Warrander¹; David Baker¹; Neil Loftus¹; Simon Hird²; ¹*Shimadzu, Manchester, UK*; ²*The Food and Environment Agency, York, UK*
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- TP 288 **Ion Mobility Spectrometry and Tandem Mass Spectrometry for the Characterization of Ganglioside Lipids from Mouse Brain Tissue using Vacuum Ionization;** Corinne Lutomski¹; Tarick El-Baba¹; James Wager-Miller²; Ken Mackie²; Sarah Trimpin¹; ¹*Wayne State University, Detroit, MI*; ²*Indiana University, Bloomington, IN*
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- TP 293 **Improved Neutral Steroids Detection and Evidence for Their Regiospecific Decompositions using Anion Attachment Mass Spectrometry;** Quentin Dumont¹; Nalaka Rannulu²; Isabelle Bailloux³; Corinne Buisson³; Nathalie Mechin³; Françoise Lasne³; Richard B. Cole¹; ¹*Université Pierre et Marie Curie, Paris, FRANCE*; ²*Johnson & Johnson, Philadelphia, PA*; ³*Agence Française de Lutte contre le Dopage, Châtenay-Malabry, France*
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- TP 312 **The Metabolic Profiling and Toxicity Study of Maleic Acid in Sprague-Dawley Rats following a Four-Week Oral Gavage Exposure;** Hsin-Chang Chen¹; Yee-Soon Ling¹; Charlene Wu¹; Su-Yin Chiang²; Kuen-Yuh Wu^{*1}; ¹National Taiwan University, Taipei, Taiwan; ²China Medical University, Taichung, Taiwan
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- TP 321 **Reconfirmation of the "Charge-Localization Isomers" of Dibasic Acids using Another GAG Disaccharide;** Yoko Ohashi¹; Yuya Otsuka²; Toshikazu Minamisawa²; Takashi Hirano¹; ¹The University of Electro-Communications, Chofu, Tokyo, Japan; ²seikagaku Corporation, Higashiyamato-Shi, Tokyo, Japan
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- TP 329 **Separation and Structural Characterization of Epimeric Mixtures of Chondroitin and Dermatan Sulfate GAGs using Field Asymmetric Ion Mobility Spectrometry (FAIMS);** Muchena J. Kailemia¹; Isaac Agyekum¹; Melvin A. Park²; Robert J. Linhardt³; Lingyun Li³; Jon Amster¹; ¹University of Georgia, Athens, GA; ²Bruker Daltonics, Inc., Billerica, MA; ³Rensselaer Polytechnic University, Troy, NY
- TP 330 **A Rapid Method to Distinguish 2,3 and 2,6-sialic Acid without Chemical Labeling and Enzyme Treatment;** Chein-Hung Chen; Ya-Ping Lin; Jung-Lee Lin; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- TP 331 **Separation and Quantitation of N-glycans with Different Sialic Acid Linkages;** Shujuan Tao¹; Yining Huang¹; Barry Boyes^{1,2}; Ron Orlando¹; ¹University of Georgia, Athens, GA; ²Advanced Materials Technology Inc, Wilmington, DE
- TP 332 **Human Platelet Function and Stability: Sequential Mass Spectrometry (MSn) and Spectrum-matching Applied to Glycomic Structure Elucidation;** Andrew Hanneman^{1,2}; David Ashline^{1,2}; Hailong Zhang¹; Melissa Lee³; Joseph Lau³; Renata Grozovsky⁴; Karin Hoffmeister⁴; Vernon Reinhold¹; ¹Glycomics Center, University of New Hampshire, Durham, NH; ²Glycan Connections, Durham, NH; ³Roswell Park Cancer Institute, Buffalo, NY; ⁴Brigham and Women's Hospital and Harvard Medical, Boston, MA
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- TP 364 **IRMPD Spectroscopy Reveals a Novel Rearrangement Reaction for Modified Peptides that involves Elimination of the N-terminal Amino Acid;** Khiry Patterson¹; John K. Gibson²; Giel Berden³; Jos Oomens³; Michael J. Van Stipdonk¹; ¹*Duquesne University, Pittsburgh, PA*; ²*Lawrence Berkeley Laboratory, Berkeley, CA*; ³*Radboud University Nijmegen, Nijmegen, The Netherlands*
- TP 365 **Fragmentation Chemistry of Asparagine and Glutamine Containing Peptides by IRMPD Spectroscopy;** Josipa Grzetic; Jonathan Martens; Giel Berden; Jos Oomens; *Radboud University Nijmegen, Nijmegen, Netherlands*
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- TP 371 **Action Spectroscopy of Protonated Pyridines and Diazines: Vibronic Detail and Product Characterization;** Christopher S. Hansen¹; Stephen J Blanksby²; Adam J. Trevitt¹; ¹*School of Chemistry, University of Wollongong, Australia*; ²*Central Analytical Research Facility, Queensland University of Technology, Australia*
- TP 372 **Probing Mobility Selected Isomers: Selective Ion-Molecule Reactions and Wavelength-Specific IR Activation;** Oscar Hernandez¹; Samantha Isenberg²; Vincent Steinmetz¹; Gary L. Glish²; Philippe Maitre¹; ¹*Université Paris Sud, Orsay, France*; ²*University of North Carolina, Chapel Hill, NC*

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- TP 383 **Ionization Characteristics of Amino Acids in Direct Analysis in Real Time-Mass Spectrometry (DART-MS);** Kanako Sekimoto¹; Motoshi Sakakura²; Takatomo Kawamukai²; Hiroshi Hike²; Teruhisa Shiota²; Fumihiko Usui²; Yasuhiko Bando²; Mitsuo Takayama¹; ¹*Yokohama City University, Yokohama, Japan*; ²*AMR, Inc., Tokyo, Japan*
- TP 384 **High-Mass Cluster Ions of Ionic Liquids in Positive-Ion and Negative-Ion DART-MS and their Application for Wide Range Mass Calibrations;** Jurgen Gross; *Organisch-Chemisches Institut, Heidelberg, Germany*
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- TP 399 **Ambient Detection of Chelation Complexes of Metals from Solids using Electrospray Laser Desorption Ionization Mass Spectrometry**; Christopher Shiea¹; Yi-Lun Chen²; Yeou-Lih Huang¹; Min Zong Huang²; ¹*Dept. of Medical Lab Sci. & Biotech., KMU, Kaohsiung, Taiwan*; ²*Dep. of Chemistry National Sun Yat-Sen University, Kaoshiung, Taiwan*
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- TP 401 **Desorption Atmospheric Pressure Photoionization-High Resolution Mass Spectrometry Fingerprinting of Urinary Steroids during Pregnancy**; Anu Vaikkinen¹; Tiina J Kauppila¹; Josef Cvacka²; Risto Kostianen¹; ¹*University of Helsinki, Helsinki, FINLAND*; ²*Institute of Organic Chemistry and Biochemistry, v. Praha, CZECH REPUBLIC*
- TP 402 **On-line Breath Analysis of VOCs in Breath using Atmospheric Pressure Chemical Ionisation with a Compact Quadrupole Mass Spectrometer**; Matthew Turner; Liam Heaney; Kayleigh Arthur; Dorota Ruskiewicz; Colin Creaser; Paul Thomas; James Reynolds; *Loughborough University, Loughborough, UK*
- TP 403 **Development of a Digital Microfluidic-Surface Acoustic Wave Nebulization Affinity Chip for MS Analysis**; Yue Huang¹; Michael Wilson¹; Scott Heron¹; John S. Edgar²; Sung Hwan Yoon¹; Patrick Langridge-Smith³; David Goodlett¹; ¹*University of Maryland, Baltimore, MD*; ²*Deurion, LLC, Seattle, WA*; ³*University of Edingburgh, edingburgh, UK*
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- TP 407 **Internal Energy Deposition for Ultrafast Laser Vaporization and Electrospray Postionization Using Thermometer Ions and Peptides**; Paul Flanigan; Fengjian Shi; Johnny Perez; Santosh Karki; Conrad Pfeiffer; Robert Levis; *Temple University, Philadelphia, PA*
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- TP 412 **Directed Proteomics of DNA-Binding Proteins;** Linda Nagore; Harry Jarrett; *UT San Antonio, San Antonio, TX*
- TP 413 **Comparative Study of the Efficiency of Different Matrices for the Analysis of Microalgae Intact Cells by MALDI TOF TOF Technique;** Lidiane Maria de Andrade¹; Maria Anita Mendes¹; Claudio Augusto Oller do Nascimento¹; Paul Kowalski²; ¹Chemical Engineering Department of POLI/USP, Sao Paulo, Brazil; ²Bruker Daltonics, Billerica, MA
- TP 414 **Anthracene-9-carbonitrile Matrix for MALDI-MS of Polyoxoanions;** Jean Boulicault; Sandra Alves; Richard B. Cole; *Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*
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- TP 416 **Increased Survival Yields of Labile Molecules using New Electron Transfer MALDI Matrices;** Laura Castellanos¹; Brian Castro²; Hernando Rosales¹; Cesar Sierra²; Cristian Blanco¹; Marianny Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Universidad Nacional de Colombia, Bogota, Colombia
- TP 417 **Homogeneous MALDI Sample Spots of Synthetic Polymers using Ionic Liquid Matrices;** Stefan J. Gabriel¹; Steffen M. Weidner¹; Clemens Schwarzwinger²; Ulrich Panne¹; ¹Fed.Inst.f.Mat.Research, Berlin, DE; ²Johannes Kepler University, Linz, AT
- TP 418 **On the Way to Quantification of Endogenous Lipids by MALDI MSI: a Practical Study of Crucial Sample Preparation Parameters;** Laure Jadoul; Rémi Longuespée; Delphine Debois; Gauthier Epepe; Edwin De Pauw; *Mass Spectrometry Laboratory, University of Liège, Liège, Belgium*
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- TP 421 **Characterization of a Distinct 1-D Gel Band from Ultracentrifuge-Enriched Exosomes;** Jeongkwon Kim¹; Zhijing Tan²; Jianhui Zhu²; Haidi Yin²; Song Nie²; David M. Lubman²; ¹Chungnam National University, Daejeon, South Korea; ²University of Michigan, Ann Arbor, U.S.A
- TP 422 **Probing the Role of APOE in Global Proteomic Changes of Cerebrospinal Fluid in Preclinical Alzheimer's Disease;** Jingxin Wang; Ozioma Okonkwo; Lingjun Li; *UW-Madison, Madison, WI*
- TP 423 **Proteomics Profiling of Pediatric Serum and Discovery of Biomarkers for Differentiation of the Cause of Febrile Illnesses in Madagascar;** Laetitia Cortes¹; Yiyong Zhou¹; Melina Messaoudi⁴; Muriel Maeder²; Rudolf Guilbaud¹; Michael Schirm¹; Jonathan Hoffmann⁴; Bénédicte Contamin²; Martin Randriamarotia³; Valentina Picot⁴; Glauca Paranhos-Baccalà⁴; Eustache Paramithiotis¹; ¹Caprion, Montreal, CANADA; ²Centre d'Infectiologie Charles Mérieux (CICM), Antananarivo, Madagascar; ³Fondation Médicale d'Ampasimanjeva (FMA), Ampasimanjeva, Madagascar; ⁴Emerging Pathogens Laboratory, Fondation Mérieux, Lyon, France
- TP 424 **Lipidomic and Transcriptomic Profiling in Mental Disease;** Raissa Lerner; Beat Lutz; Laura Bindila; , Mainz, Germany
- TP 425 **Iron Modified Peptides as Biomarkers of Gynecologic Malignancies;** Meghan Tanner; Lindsay Schambeau; Michael Finan; Rodney Rocconi; Lewis Pannell; *Mitchell Cancer Institute, Mobile, AL*
- TP 426 **Improved Detection and Quantification in Plasma-based Biomarker Discovery;** Michael Burgess¹; Hasmik Keshishian¹; D.R. Mani¹; Philipp Mertins¹; Karl Clauser¹; Michael A. Gillette^{1,2}; Robert Gerszten^{1,2}; Steven A. Carr¹; ¹Broad Institute, Cambridge, MA; ²Massachusetts General Hospital, Boston, MA
- TP 427 **Comparing Ion Thermal Focusing Electrospray and Nanospray LC-MS/MS for Characterizing Human Embryonic Stem Cells and Neural Progenitor Cells;** Raghothama Chaerkady¹; Vadiraja Bhat²; Dawn Stickle²; Robert Giuffre²; Hyesoo Kim¹; Robert N Cole¹; Candace L Kerr³; ¹Johns Hopkins University School of Medicine, Baltimore, MD; ²Agilent Technologies, Wilmington, DE; ³University of Maryland, Baltimore, MD
- TP 428 **Evaluation of Multiple Search Engines for the Proteomic Analysis of Pap Tests for Biomarker Discovery in Gynecological Malignancies;** Somi Afiuni; Kristin Boylan; Timothy Griffin; Amy Skubitz; *University of Minnesota, Minneapolis, MN*
- TP 429 **Proteomic Investigation of Saliva from Children with Autism Spectrum Disorder and Matched Controls by SDS-PAGE and DIGE and LC-MS/MS;** Katherine Beglinger¹; Kelly Wormwood¹; Armand Ngounou¹; Jeanne Ryan²; Costel Darie¹; Alisa G. Woods¹; ¹Clarkson University, Potsdam, NY; ²SUNY, Plattsburgh, NY
- TP 430 **Multiplexed Protein Expression Profiling of Pancreatic Stellate Cells under Nicotine Stress;** Joao Paulo; Steven Gygi; *Harvard Medical School, Boston, MA*
- TP 431 **Application of iTRAQ Proteomics to Study Biotherapeutic mAb Production in CHO Cells;** Deniz Baycin Hizal¹; David Gold¹; Huifang Dong¹; Wei Zhu¹; Raghothama Chaerkady²; Robert Cole²; Herren Wu¹; Michael Bowen¹; Jie Zhu¹; ¹MedImmune, Gaithersburg, MD; ²Johns Hopkins University, Baltimore, MD
- TP 432 **Metabolic Profiling of Transgenic Mouse Model for Polyp-Stage Colorectal Cancer;** Michael Williams¹; Xing Zhang¹; Amy Belton²; Jeong-Jin Park¹; William Siems¹; David Gang¹; Linda Resar²; Raymond Reeves¹; Herbert Hill¹; ¹Washington State University, Pullman, Washington; ²Johns Hopkins University School of Medicine, Baltimore, MD
- TP 433 **Application of Mass Spectrometry for Tumor Proteogenomic Signature Discovery;** Michael C. Wendl¹; Song Cao¹; R. Jay Mashl¹; Kelly Ruggles⁴; Philipp Mertins⁵; Pei Wang⁶; Harsha Gunawardena⁷; John Wrobel¹; Beifang Niu¹; Kai Ye¹; Matthew A. Wyczalkowski¹; Michael McLellan¹; Christopher A. Maher^{1,2}; Sherri R. Davies²; R.

- Reid Townsend²; David Fenyó⁴; Steven A. Carr⁵; Xian Chen⁷; Matthew J. Ellis^{2,3}; Li Ding^{1,2}; ¹The Genome Institute at Washington University, St. Louis, MO; ²Washington University Dept of Medicine, St. Louis, MO; ³Siteman Cancer Center, St. Louis, MO; ⁴NYU Langone Medical Center, New York, NY; ⁵Broad Institute, Cambridge, MA; ⁶Fred Hutchinson Cancer Research Center, Seattle, WA; ⁷UNC School of Medicine, Chapel Hill, NC
- TP 434 **Investigating Post-Transcriptional Modifications of Viral RNA by Affinity Capture and MS Analysis;** W. McIntyre¹; Rebecca E. Rose¹; M. Arra²; M. Canki²; C. Pager¹; D. Fabris¹; ¹The RNA Institute, University at Albany, Albany, NY; ²Albany Medical Center, Albany, NY
- TP 435 **Proteins Regulated by Shear Stress (SS) Intensity and Their Correlation with Atherosclerosis;** Gabriela Venturini¹; Rafael Dariolli¹; Jéssica Silva Salgueiro²; Karina Helena Morais Cardozo²; Valdemir Melechco Carvalho²; José Eduardo Krieger¹; Alexandre da Costa Pereira¹; ¹Heart Institute - FMUSP, Sao Paulo, SP - Brazil; ²Fleury Group, São Paulo, SP - Brazil
- TP 436 **Understanding the Effect of Cysteine on Proteomic Profiles in *Saccharomyces cerevisiae* with High Consistency and Accuracy using Data Independent Acquisition;** Ajay Bhat^{1,2}; Trayambak Basak^{1,2}; Dipankar Malakar³; Manoj Pillai³; Shantanu Sengupta^{1,2}; ¹CSIR-Institute of Genomics and Integrative Biology, New Delhi, India; ²Academy of Scientific and Innovative Research, New Delhi, India; ³AB Sciex, India, Gurgaon, India
- TP 437 **Label-free Quantitative Analysis of Radiation-induced Differential Protein Expression in The Mouse Lung Proteome;** Bao Quoc Tran¹; Young Ah Goo¹; Catherine Booth²; Greg Tudor²; Wenjing Li¹; David R. Goodlett¹; Thomas J. MacVittie¹; Maureen A. Kane¹; ¹University of Maryland, Baltimore, MD; ²Epistem Ltd, Maschester, UK
- TP 438 **Integrated Phosphoproteogenomic Analyses of Patient-Derived Breast Cancer Xenograft Models Allow Molecular Characterization of Human Disease Biology and Therapeutic Response;** Michael A. Gillette^{1,2}; Philipp Mertins¹; Jana W. Qiao¹; D. R. Mani¹; Karl R. Clauser¹; Sherri R. Davies⁵; Kelly V. Ruggles³; Song Cao⁵; Christopher A. Maher⁶; Michael McLellen⁵; David Fenyó⁴; Li Ding⁵; Matthew J. Ellis⁵; Steven A. Carr¹; ¹Broad Institute of Harvard and MIT, Cambridge, MA; ²Massachusetts General Hospital, Boston, MA; ³NYU Langone Medical Center, New York, NY; ⁴New York University, New York, NY; ⁵Washington University, St. Louis, Missouri
- TP 439 **Deciphering Systemic Responses to Brain Disorders by Quantitative Proteomics;** Li Cao; Fang Bian; An Zhou; ^{Morehouse school of medicine, Atlanta, GA}
- TP 440 **Robotic Preparation of Hundreds of Clinical Samples for Protein Biomarker Verification and Validation;** Tony Tegeler¹; Matthew Rosenow¹; Paul Russo²; Ruben Magni²; Alessandra Luchini²; Lance Liotta²; Emanuel Petricoin²; Patrick Pirrotte¹; ¹Translational Genomics Research Institute, Phoenix, AZ; ²Center for Applied Proteomics & Molecular Medicine, Manassas, VA
- TP 441 **Discovery of Tissue Regenerating Biomarkers in the Secretome Released from Human Embryonic Stem Cell-derived Hepatocytes by Using Proteomic Approach;** Hee-Joung Lim^{1,2}; Jiyoun Han¹; Yu Jin Jang¹; Ae Eun Seok²; Jong-Moon Park³; Hyun-Jin Jung⁴; Yong-Seung Shin⁴; HooKeun Lee³; Jong-Hoon Kim¹; Hee-Gyoo Kang²; ¹Laboratory of Stem Cells, Korea University, Seoul, Republic of Korea; ²Bio-medical Laboratory, Eulji University, Seongnam, Republic of Korea; ³Laboratory of Proteomics, Gachon University, Incheon, Republic of Korea; ⁴Agilent technologies Ltd, Suwon, Republic of Korea
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- TP 444 **PZP as a Novel Biomarker for Early Alzheimer's Disease;** Diana A.T. Nijholt; A. Ikram; J.M. Kros; P.A.E. Sillevius Smitt; P.J. Koudstaal; T.M. Luider; ^{Erasmus Medical Centre, Rotterdam, Netherlands}
- TP 445 **Biomarker Discovery in Cerebrospinal Fluid for Schizophrenia and Antipsychotic Drug Treatment-Induced Weight Gain;** Geun-Cheol Gil¹; Bich Nguyen¹; Yiyong Zhou²; Xiaolei Xie¹; Rene Allard²; Howard Schulman¹; Daniel Chelsky¹; Sushmita Mimi Roy¹; ¹Caprion Proteomics US LLC, Menlo Park, CA; ²Caprion Proteomics Inc, Montreal, Canada
- TP 446 **Elucidation of Epileptogenic Mechanisms using a Mass Spectrometry-Based Metabolomics Approach;** Svenja Heischmann¹; Kevin Quinn²; Charmion Cruickshank-Quinn²; Lindsey B. Gano¹; Joe Gomez¹; Nicole Reisdorph²; Manisha Patel¹; ¹University of Colorado Denver, School of Pharmacy, Aurora, CO; ²National Jewish Health, Denver, CO
- TP 447 **Profiling Urinary Proteome for Stress Induced Female Urinary Incontinence;** Marianne Koch²; Rosa Laterza²; Wei-Qiang Chen¹; Miloš Barut³; Sonja Seyfert⁴; Heinz Kölbl²; Goran Mitulovic¹; ¹Medical University of Vienna, KIMCL, Vienna, Austria; ²Medical Univ of Vienna, Dept. of Gyn. and Obst., Vienna, Austria; ³BIA Separations, Ajdovščina, Slovenia; ⁴Medical Univ of Vienna, Proteomics Core Facility, Vienna, Austria
- TP 448 **Immuno-based-LC/SRM as a Diagnostic tool for Measuring Protein Dynamics of Amyloid β Isoforms Instead of ELISA in the Clinical Laboratory;** Kwasi Mawuenyega; Tom Kasten; Vitaliy Ovod; Brendan Lucey; Wendy Sigurdson; Randall Bateman; ^{Washington University School of Medicine, Saint Louis, MO}
- TP 449 **Proteome Analysis of Exhaled Breath Condensate for Lung Cancer Biomarker Discovery;** NL Starodubtceva^{1,3}; AM Ryabokon¹; AS Kononikhin^{2,3}; EN Kukaev^{1,2}; IA Popov^{1,2}; VA Bagrov⁴; OV Pikin⁴; VV Barmin⁴; EC Anaev⁵; SD Varfolomeev¹; EN Nikolaev^{1,2}; ¹Emanuel Institute of Biochemical Physics, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Research Center for Obstetrics, Gynecology, Moscow, Russia; ⁴Gertsen Institute of Oncology, Moscow, Russia; ⁵Research Institute of Pulmonology, Moscow, Russia
- TP 450 **Analysis of Extracellular Matrix Peptides in Chronic Obstructive Pulmonary Disease (COPD) by LC/MS;** Jiangtao He^{1,1}; Shuren Ma¹; Yong Y Lin¹; Jerome Cantor²; Gerard Turino¹; ¹Icahn School of Medicine at Mount Sinai, New York, NY; ²St. John's University, New York, NY
- TP 451 **The Mitochondrial Deacetylase SIRT3 is a Host Defense Factor Hijacked during Viral Infection;** Rommel Mathias; Matthew Lefebvre; Ileana M. Cristea; ^{Princeton University, Princeton, NJ}

- TP 452 **Investigation on Redox Metabolism and Dopaminergic Cell Death in Response to Neuron Toxins by a MS and NMR Combined Technique;** Shulei Lei; Darrell Marshall; Yuting Huang; Aracely Garcia-Garcia; Renu Nandakumar; Eric Dodds; Rodrigo Franco; Robert powers; *university of nebraska lincoln, lincoln, NE*
- TP 453 **Defining the Exposome: a Critical Quantity to Determine the Causes of Chronic Human Disease;** Anthony Macherone^{1,2}; ¹*Agilent Technologies, Inc., Wilmington, DE*; ²*Johns Hopkins University, Baltimore, MD*
- TP 454 **Identification of Potential Metabolite Biomarkers of Lower Urinary Tract Symptoms (LUTS) in Mouse and Human Urines;** Ling Hao¹; Tyler Greer²; Chad Vezina³; Will Ricke⁴; Paul Marker¹; Dale Bjorling³; Wade Bushman⁴; Lingjun Li^{1,2}; ¹*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; ²*Department of Chemistry, UW-Madison, Madison, WI*; ³*School of Veterinary Medicine, UW-Madison, madison, WI*; ⁴*Department of Urology, UW-Madison, madison, WI*
- TP 455 **A quantitative LC-MS/MS (Qtrap) Method to Profile Sphingolipids in Pancreatic β -cells;** Kumari Ubhayasekera; Bo EK; Jonas Bergquist; *Uppsala University, Uppsala, Sweden*
- TP 456 **Differential Accumulation of Glycosphingolipids in a Tay-Sachs Disease Brain;** Huan He¹; Yu-Teh Li²; Su-Chen Li²; Nicolas L. Young¹; Alan G. Marshall^{1,3}; ¹*Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*; ²*Tulane University School of Medicine, New Orleans, LA*; ³*Department of Chemistry and Biochemistry, FSU, Tallahassee, FL*
- TP 457 **Quantitative Phosphoproteomic Phenotyping of Acquired Resistance to HER2 Kinase Inhibitors in Breast Cancer using Multimodal Phosphopeptide Enrichments;** Erik J. Soderblom¹; Hongbo Gu²; Jeffrey Sliva²; J. Will Thompson¹; Wenle Xia¹; Neil Spector¹; M. Arthur Moseley¹; ¹*Duke University School of Medicine, Durham, NC*; ²*Cell Signaling Technology, Danvers, MA*
- TP 458 **Proteomics Study of SCYL2-Knockdown Effect on the Distribution of Amyloid Precursor Protein and Its Fragments in the APP-Overexpressing N2a Cells;** Ko-Yi Chien; Rong Wang; *Icahn School of Medicine at Mount Sinai, New York, NY*
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- TP 459 **A Sensitive Isotopic Dilution LC/MS Methodology to Evaluate Asymmetric Dimethyl Arginine Levels as a Plasma Biomarker of Endothelial Function;** Jose Castro-Perez; Paul Miller; Sheng-Ping Wang; Dan Xie; Stephen Previs; Doug Johns; *Merck Research Laboratories, Kenilworth, NJ*
- TP 460 **Quantification of Intact and Truncated Stromal cell-derived factor-1 α (SDF-1 α) in Circulation by Immunoaffinity Enrichment and Tandem Mass Spectrometry;** Weixun Wang¹; Bernard Choi¹; Wenyu Li¹; Julie Lao¹; Anita Lee¹; Sandra Souza¹; Nathan Yates²; Timothy Kowalski¹; Alessandro Poci³; Lucinda Cohen¹; ¹*Merck Research Labs, Rahway, NJ*; ²*University of Pittsburgh, Pittsburgh, PA*; ³*Janssen R&D, Spring House, PA*
- TP 461 **Detection of Endothelial Cell Surface Proteins following Irradiation as Potential Targets for Brain Arteriovenous Malformations Molecular Therapy;** Margaret Simonian; *UCLA, Los Angeles, CA*
- TP 462 **Measuring Protein Analyte Panels in Dried Blood Spots (DBS) using an Automated SISCAPA-MS Workflow;** Morteza Razavi¹; Leigh Anderson¹; Selena Larkin¹; Terry Pearson^{1,2}; ¹*SISCAPA Assay Technologies, Washington, DC*; ²*University of Victoria, Victoria, BC Canada*
- TP 463 **Quantitative Activity-Based Kinase Profiling in Lung Cancer;** Bin Fang; Jiannong Li; Elizabeth Wood; Y. Ann Chen; Stephen Brantley; Fumi Kinose; Wei Guan; Andrew Myers; Steven Eschrich; Uwe Rix; Eric Haura; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- TP 464 **Determination of Urea in Human Serum and Epithelial Lining Fluid Using LCMS; Benchmarking to a Traditional Diagnostic Colorimetric Kit;** Christopher A Evans; Chester L Bowen; Amanda Watkins; Bonnie Orr; *GlaxoSmithKline, King Of Prussia, PA*
- TP 465 **Investigation of Angiotensin Biomarker Dynamics Employing Micro-Flow LC and Microfluidic ESI-MS;** Thomas Mencken; Jonathan Kehler; Matthew Szapacs; Chester Bowen; *GlaxoSmithKline, Collegeville, PA*
- TP 466 **Cross-Validation of a Ligand Binding and Immunocapture / LC-MS Assay for the Determination of the Biomarker Periostin;** Jonathan Kehler; Matthew Szapacs; *GlaxoSmithKline, King Of Prussia, PA*
- TP 467 **Targeted MS2 Quantitation of Exon Skipping Restored Dystrophin in a Mouse Model of Duchenne Muscular Dystrophy;** Kristy J. Brown; Kitipong Uaesoontrachoon; Aiping Zhang; Conner Shaughnessy; Ramya Marathi; Sree Rayavarapu; Maria Candida Vila; Eric Hoffman; Kanneboyina Nagaraju; Yetrib Hathout; *Children's National Health System, Washington, DC*
- TP 468 **An Omics study of CSF from HAND patients under cART reveals evidence for macrophage activation and perturbations in glutamate metabolism;** Adriana Bora¹; Ceereena Ubaida Mohien¹; Alexey Lyashkov³; Anne Blackwell²; Linda Chang⁴; Richard IV Moxley¹; Ned Sacktor¹; Justin C. McArthur¹; Norm Haughey¹; Avindra Nath³; David R. Graham¹; ¹*Johns Hopkins Medical School, Baltimore, MD*; ²*Agilent Technologies, Santa Clara, CA*; ³*National Institute of Health, Bethesda, MD*; ⁴*Hawaii University, Honolulu, HI*
- TP 469 **Simultaneous Quantitation of Neurotransmitters in Dialysates Using LC/MS-MS;** Shiling Jia; Fan Wang; Charles Yang; Wei Tang; Alicia Y Du; *Chempartners, Shanghai, Zhang, Jiang, China*
- TP 470 **Development of a Multiplexed Targeted SRM Assay for NCI's Top Tumor Associated Antigens for Biomarker Screening in Multiple Cancer Types;** Erik J. Soderblom; Lisa St. John - Williams; Wenle Xia; Meredith E. Turner; Matthew W. Foster; Neil Spector; M. Arthur Moseley; *Duke University School of Medicine, Durham, NC*
- TP 471 **Discovery and Verification of Neurotrauma Markers by High Mass Accuracy/High Resolution Mass Spectrometry;** Sean Shen¹; Ina Wanner²; Joseph A. Loo¹; ¹*Department of Chemistry and Biochemistry, Los Angeles, CA*; ²*Semel Institute for Neuroscience & Human Behavior, Los Angeles, CA*
- TP 472 **Sequence Quantitative Analysis (SEQUANA): targeted-Proteomic Method for Accurate Alzheimer's Disease Diagnostic by CSF Tau Proteoforms Monitoring;** Nicolas Barthélemy^{1,2}; Christophe Hirtz²; François Fenaille¹; Susanna Schraen-Maschke³; Audrey Gabelle²; Christophe Junot¹; Sylvain Lehmann²; François Becher¹; ¹*CEA Saclay, DSV/iBiTec-S/LEMM, Gif s/Yvette, France*; ²*CHU Montpellier, Hôpital St Eloi, IRMB/LBPC, Montpellier, France*; ³*Inserm, UMR 837, IMPRT, Faculté de Médecine, Lille, France*
- TP 473 **ATP7B Analysis by Immuno-SRM-MS for Wilson Disease;** Sunhee Jung; Si Houn Hahn; *Seattle Children's, Seattle, WA*
- TP 474 **Development of a LC-MS/MS Method to Biomonitor 1,3-Butadiene Exposure and Early Biological Effects in Nonsmokers and Smokers;** Xiaotao Zhang^{1,2}; Hongwei

- Hou¹; Longkai Shi¹; Yong Liu²; An Wang²; Qingyuan Hu¹; ¹China National Tobacco Quality Supervision & Test, Zhengzhou, CHINA; ²Anhui Institute of Optics and Fine Mechanics, Hefei, China
- TP 475 **Simultaneous Determination of N3-methyladenine, N3-ethyladenine and N3-(2-hydroxyethyl)adenine in Human Urine by Liquid Chromatography-Tandem Mass Spectrometry**; Yongfeng Tian¹; Hongwei Hou¹; Xiaotao zhang¹; An Wang²; Yong Liu²; Qingyuan Hu¹; ¹China National Tobacco Quality Supervision & Test, Zhengzhou, China; ²Anhui Institute of Optics and Fine Mechanics, Hefei, China
- TP 476 **Variability of Urinary VOC Metabolites Concentration in Before Bed, First Morning Void, and Spot Urine Samples**; Deepak Bhandari¹; K. Udeni Alwis¹; B. Rey deCastro¹; Connie Sosnoff¹; Yu Qiu¹; Marsha Morgan²; Jon Sobus²; Benjamin Blount¹; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²US Environmental Protection Agency, Research Triangle Park, NC
- TP 477 **Identification and Quantitation of N-glycans in Dyssynchronous Heart Failure**; Shuang Yang¹; Lijun Chen¹; Punit Shah¹; Jonathan Kirk²; David A. Kass²; Jennifer E. van Eyk³; Hui Zhang¹; ¹John Hopkins Dept. of Pathology, Baltimore, MD; ²Johns Hopkins Cellular and Molecular Medicine, Baltimore, MD; ³Johns Hopkins Institute for Computational Medicine, Baltimore, MD
- TP 478 **Automated Extraction of Glycans and Peptides for Glycomic and Proteomic Analyses**; Jing Chen; Shuang Yang; Hui Zhang; Johns Hopkins University, Baltimore, Maryland
- TP 479 **Utilizing Online Extraction Techniques to Increase Sensitivity and Improve Sample Preparation Efficiency for Quantitative LCMS: A cGMP Biomarker Case Study**; Elisabeth Lonie; Dawn Dufield; Pfizer, Andover, MA
- TP 480 **Accurate Quantitation of Endogenous Compounds by Standard Addition Amended Calibration (SAAC) in Matched Matrix**; Zhenmin Liang; John Hanley; Lisa Borbridge; Allergan, Irvine, CA
- TP 481 **Comparison of Label-Free and Label-Based Strategies for Proteome Analysis of Hepatoma Cell Lines**; Dominik Andre Megger¹; Leona Louise Pott¹; Kristin Rosowski¹; Birgit Korte¹; Don Marvin Voss¹; Stephanie Tautges¹; Thilo Bracht¹; Maike Ahrens¹; Juliet Padden¹; Martin Eisenacher¹; Katja Kuhlmann¹; Helmut E. Meyer^{1,2}; Barbara Sitek¹; ¹Ruhr-Universitaet Bochum, MPC, Bochum, Germany; ²Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany
- TP 482 **Quantitative Analysis of the PTEN-Induced Kinase (Pink-1) Mutant in C. elegans using Tandem Mass Tags**; Geert Baggerman^{1,2}; Dirk Valkenborg^{1,2}; Evelyne Maes^{1,3}; Karin Schildermans²; Inge Mertens^{1,2}; ¹VITO, Mol, Belgium; ²CFP-CeProMa, University of Antwerp, Antwerp, Belgium; ³Functional Genomics and Proteomics lab, Leuven, Belgium
- TP 483 **Identification of Protein Biomarkers for the Cellular Response to Proteasome Inhibition using a Simple, Robust Platform Enabling Proteome-Wide, Label-Free Quantification**; Aaron Aslanian^{1,2}; Xuemei Han¹; John Yates III¹; ¹The Scripps Research Institute, La Jolla, CA; ²Salk Institute for Biological Studies, La Jolla, CA
- TP 484 **Development and Application of a Quantitative Proteomic Method for Verification of Neurodegenerative-related Biomarkers in Human CSF**; Andrew Percy¹; Juncong Yang¹; Andrew Chambers¹; Romain Simon¹; Darryl Hardie¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- TP 485 **Improving Selectivity and Sensitivity in Clinical Assays using Parallel Reaction Monitoring**; Bruno Domon¹; Sebastien Gallien¹; Yeoun-Jin Kim¹; Guy Berchem²; ¹Luxembourg Clinical Proteomics Center, Strassen, Luxembourg; ²CRP-Sante, Strassen, Luxembourg
- TP 486 **High Sample Throughput SISCAPA-UMRM MS Quantitation of Prostate Specific Antigen in Nondepleted Serum**; Mary Joan Castillo; Adam Mcshane; Min Cai; Alexander Gomes; Xudong Yao; University of Connecticut, Storrs, CT
- TP 487 **An Alternative Computational Solution to Protein Quantitation in Plasma Proteome Analysis using LC-MS/MS with Travelling Wave Ion Mobility**; Charlotte E. Daly; Leong L. Ng; Amirmansoor Hakimi; Richard Willingale; Donald J.L. Jones; University of Leicester, Leicester, UK
- TP 488 **Impaired Regulation of Tyrosine Phosphorylation in Skeletal Muscle in Type 2 Diabetes**; Danjun Ma¹; Berhane Seyoum¹; Michael Caruso¹; Zaher Msallaty¹; Monique Lewis¹; Chengjian Tu²; Michael Diamond¹; Abdul About-Samra¹; Xiangmin Zhang¹; Wissam Al-janabi¹; Rodney Berry¹; Kurt Højlund³; Jeffrey Horowitz⁴; Rebecca Tagett Tagett¹; Sorin Draghici¹; Zhengping Yi¹; ¹Wayne state university, Detroit, MI; ²University at Buffalo, Buffalo, NY; ³Odense University Hospital, Odense, Denmark; ⁴University of Michigan, Ann Arbor, MI
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- TP 489 **Application of Novel Pre-Charged and Highly Specific Fluorinated Azide for the Trace Analysis of Ethinylestradiol using Copper-Catalyzed Click Reaction**; Priyanka Chitranshi; Lucie Loukotkova; Goncalo Gamboa Da Costa; US-FDA/NCTR, Jefferson, AR
- TP 490 **On-Line Pre-Treatment and Quantification of Trace Estrogens in Serum by Bulk Derivatization and Direct Cation ExchangeTrap-and-Elute LC/MS/MS**; Liangqiao Bian^{1,2}; Jana Chalupová^{4,5}; Hui Fan³; Marek Šebela^{4,5}; Maciej Kukula^{1,2}; Joe Barrera²; Kevin A. Schug³; ¹Shimadzu Center for Advanced Analytical Chemistry, The University of Texas at Arlington, Arlington, TX; ²Shimadzu Institute for Research Technologies, The University of Texas at Arlington, Arlington, TX; ³Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; ⁴Department of Biochemistry, Palacký University, Olomouc, Czech; ⁵Department of Protein Biochemistry and Proteomics, Palacký University, Olomouc, Czech
- TP 491 **Development and Validation of LC/MS/MS Methods to Quantify EC1456 and Tubulysin B Hydrazide in Rat Plasma**; Michael Pugh; Satish Rao; Patrick J. Klein; Christopher P. Leamon; Endocyte, Inc., West Lafayette, IN
- TP 492 **Development and Qualification of a Fast and Sensitive LC-MS/MS Method for the Simultaneous Quantification of Microdosed Statins in Human Plasma**; Cynthia M. Chavez-Eng; Ryan Lutz; Dina Goykhman; Kevin Bateman; Merck & Co., West Point, PA
- TP 493 **Development of an Ultra-Sensitive, High-Throughput Multiplexed LC(HILIC)-MS/MS Method for the Simultaneous Quantitation of Naloxone, Buprenorphine, and Norbuprenorphine**; Xiaodong Zhu; Thomas Horuath; Jingguo Hou; Edward Wells; Steve Unger; Worldwide Clinical Trials Drug Development Solutio, Austin, TX
- TP 494 **Challenges in Quantification of Metal-based Oncology Drugs in Human Plasma Using Triple Quad 5500 System**; Feng Yin; Guangnong Zhang; Urszula Lorent; Emily Epure; Andrew Swenson; Yong-Xi Li; Medpace Bioanalytical Laboratories, Cincinnati, OH

- TP 495 **Simultaneously Sensitive and Accurate Measurements of Seven Steroid Hormones in Post-Menopausal Women Serum by a Robust LC-MS/MS Method;** Yuyong Ke; Renaud Gonthier; Jonathan Bertin; Fernand Labrie; *EndoCeutics Laboratory, Québec, Canada*
- TP 496 **Highly Sensitive Quantitative Estimation of Genotoxic Impurities using LC/MS/MS;** Shruti Raju; Deepti Bhandarkar; Rashi Kochhar; Shailesh Damale; Shailendra Rane; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 497 **Highly sensitive Quantitative Analysis of Felodipine and Hydrochlorothiazide from Plasma using LC/MS/MS;** Shailendra Rane; Rashi Kochhar; Deepti Bhandarkar; Shruti Raju; Shailesh Damale; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 498 **Low level Quantitation of Loratidine from Plasma using LC/MS/MS;** Shailesh Damale; Deepti Bhandarkar; Shruti Raju; Rashi Kochhar; Shailendra Rane; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 499 **High Throughput Analysis of Liquiritigenin and Isoliquiritigenin In Rodent Serum Using UPLC-Tandem Mass Spectrometry;** Nathan C. Twaddle¹; Mona I. Churchwell¹; Estatira Sepehr¹; Ashish Sawhney¹; William G. Helferich²; Daniel R. Doerge¹; ¹*NCTR/FDA, Jefferson, AR*; ²*University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 500 **An Analytical Method for Automated Analysis of Plasma Dapsone, Trimethoprim, Sulfamethoxazole, Sulfamethazine, Sulfamethizole, and Sulfathiazole for Dose Optimization;** Claudia Meek; Nyokabi Miingi; Erling Beck; Ronald Hall; Richard Leff; *Texas Tech University Health Sciences Center, Dallas, TX*
- TP 501 **LC-MS/MS Bioanalysis of Dapagliflozin and Its Glucuronide Metabolite in Human Blood Using Dried Blood Spot;** Jane Liu¹; Sophia (Xiaohui) Xu¹; Guowen Liu¹; David Boulton¹; Melanie Pe Benito¹; Marsha Epstein¹; Michael Waldron²; Pathanjali Kadiyala¹; Jim Shen¹; mark arnold¹; Qin ji¹; ¹*Bristol-Myers Squibb Co., Princeton, NJ*; ²*PPD, Richmond, VA*
- TP 502 **Determination of Pradigastat, a DGAT1 Inhibitor in Human Plasma using MicroLC-MS/MS;** Tapán Majumdar; Shari Wu; Cindy Chen; Adam Bentley; Jimmy Flarakos; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- TP 503 **Quantitative Estimation of Potential Genotoxic Impurities in Drug Development without Synthetic Standards by High Resolution Mass Spectrometer and UV Detection;** Chunang (Christine) Gu; Andrew McClory; Sarah Stowers; Jason Gruenhagen; Alan Deese; *Genentech, South San Francisco, CA*
- TP 504 **Overcoming Chiral Method Development Challenges: UPLC-MS/MS Method for Determination of Dextroamphetamine and Levoamphetamine in Human Plasma after Chiral Derivatization;** Yuwen Zhao; Vi Dan; Yuan-Shek Chen; Luca C. Matassa; *QPS, LLC, Newark, DE*
- TP 505 **Ultra-Trace Quantitation of Catechins in Human Blood Plasma to Facilitate Kinesiology Study using Restricted Access Media LC/MS/MS;** Aionna Guerrero¹; Sarah Hughes¹; Hui Fan¹; Michelle Harrison²; Kevin Schug¹; ¹*UT Arlington, Arlington, TX*; ²*UT Austin, Austin, TX*
- TP 506 **Development and Validation for the Simultaneous Determination of Emtricitabine and Tenofovir in Human Plasma by LC-MS/MS;** Jingguo Hou; Laura Binneboese; Melody Adam; Steven Hoehne; Kevin McManus; Xiaodong Zhu; Edward Wells; *WWCT, Austin, TX*
- TP 507 **Absolute Quantitation of Aminoglycoside Antibiotics in Mouse Plasma by a HILIC-based LC-MS/MS Method;** Ludmila Alexandrova¹; Allis Chien¹; Robert Greenhouse²; Anthony Ricci³; ¹*Stanford University Mass Spectrometry, Stanford, CA*; ²*SPARK, Stanford University School of Medicine, Stanford, CA*; ³*Department of Otolaryngology, School of Medicine, Stanford, CA*
- TP 508 **A Simple, Reliable and Rapid LC-MS/MS Method for Simultaneous Determination of Carbamazepine and Carbamazepine-10,11-epoxide in human plasma;** Shuyu Hou; Yuan-Shek Chen; *QPS, LLC, Newark, DE*
- TP 509 **Supercritical Fluid Chromatography-Tandem Mass Spectrometry for Fast Chiral Separation of Cetrizine in Human Plasma;** Han Young Eom; Hyun-Deok Cho; Joon Hyuk Suh; Unyong Kim; Junghyun Kim; Yura Jung; Bong-Joon Kim; Sang Beom Han; *Chung-Ang University, Seoul, South Korea*
- TP 510 **Simultaneous Quantitative Analysis of 20 Amino Acids in Food Samples without Derivatization using LC-MS/MS;** Keiko Matsumoto¹; Jun Watanabe¹; Itaru Yazawa²; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*Imtakt Corporation, Kyoto, Japan*
- TP 511 **Assay of Human Saliva Steroids by Stable Isotope Coded Derivatization (ICD) and Tandem Mass Spectrometry;** Fabio Mazzotti¹; Leonardo Di Donna¹; Domenico Taverna¹; Anna Napoli¹; Constantinos M. Athanassopoulos²; Giovanni Sindona¹; ¹*University of Calabria, Arcavacata Di Rende, Italy*; ²*University of Patras, Patras, Greece*
- TP 512 **A generic LC-MS Cleaning Verification Assay for High Potency Drugs;** Vinayak AK¹; Syed Lateef¹; Chunang (Christine) Gu²; Michael Dong²; ¹*Agilent Technologies, Bangalore, India*; ²*Genentech, South San Francisco, CA*
- TP 513 **Automated Bioanalytical Method Development for Methotrexate and Sulfasalazine Utilizing Quality-by-Design Approach;** Syed Salman Lateef; Siji Joseph; *Agilent Technologies, Bangalore, INDIA*
- TP 514 **Verification of an LC-MS/MS Method for 14 Antidepressants Utilizing Dried Blood Spots;** Kerry Hassell; Sarah Fair-Wandland; Joseph L. Herman; *ThermoFisher Scientific, Franklin, MA*
- TP 515 **Evaluation and Application of a Non-contact Digital Dispenser, HP D300, in Bioanalysis;** Debra Liao; Susan Chen; Martin Paton; Mark Qian; *Millennium: The Takeda Oncology Company, Cambridge, MA*
- TP 516 **Can DMSO Provide Benefit in Application beyond Proteomic?;** J.C. Yves Leblanc; *AB SCIEX, Concord, On, Canada*
- TP 517 **A Sensitive Method for the Determination of Lithium in Human Plasma Using ICP-MS Detection;** Patrice Lantin; Sylvain Lachance; François Viel; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- TP 518 **Compound Dependence of LC-MS-MS Flow Rate Sensitivity;** Jay Corr; Thomas Covey; *AB SCIEX, Concord, Canada*
- TP 519 **Development of a Highly Sensitive, Efficient, Combo Extraction Method for the Quantitation of Formoterol and Budesonide by UPLC/MS/MS;** Ryan S. Adler; Sherry Liu; Alicia Pietrasiewicz; Spencer J. Carter; Qiuying Zhu; Min Meng; *Tandem Labs, Salt Lake City, UT*
- TP 520 **A Simple, Selective and Highly Sensitive UPLC-MS/MS Method for Determination of Mometasone Furoate in Human Plasma;** Hao Li; Huafang Jiang; Ling Zhou; Xiaohang Shen; Jinsong Xing; Wenzhong Liang; *WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*

- TP 521 **Improving Detection Limits of Prohibited Substances and Therapeutics by Solid Phase Microextraction (SPME) Coupled to LC-MS/MS;** [Frenny Ruparella](#)¹; Lisa Cousins¹; Nathaly Reyes-Garcés²; Germán Augusto Gómez-Ríos²; Barbara Bojko²; Janusz Pawliszyn²; ¹IONICS Mass Spectrometry, Bolton, Canada; ²Department of Chemistry, University of Waterloo, Waterloo, Canada
- TP 522 **LC-MS/MS Methods Development for the Analysis of Polymeric Materials and Related Metabolites in Biological Matrices;** [Changyu Quang](#); Brett D. Dunbar; Nichole R. Myers; William C. Nethero; Michael P. Donegan; Elizabeth A. Groeber; *WIL Research, Ashland, OH*
- TP 523 **LC-MS/MS Method of Isradipine: Unsuitability of Isradipine-D3 as Internal Standard Due to Temperature-dependent Transesterification in Ion Source;** Hao Li¹; Jie Zhang²; Yan Fu¹; Changqing Lin¹; [xiaohang shen](#)¹; jinsong xing¹; Wenzhong Liang¹; ¹WuXi AppTec (Shanghai) Co. Ltd., Shanghai, CHINA; ²Novartis Institutes for BioMedical Research, East Hanover, NJ
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- TP 524 **Isomer Differentiation of Explosives-related Compounds and Clarification of the 30 Da Releases from TNT using Electrospray High-Resolution Multistage Mass Spectrometry;** [Adrián Schwarzenberg](#)¹; Richard B. Cole¹; Héloïse Dossmann¹; Xavier Machuron-Mandart²; Jean-Claude Tabet¹; ¹Université Pierre et Marie Curie, IPCM/CSOB, Paris, France; ²CEA, DAM, DIF, F-91297, Arpajon, France
- TP 525 **Understanding of Fundamental Ion Behavior Leads to Routine Substructure Identification: A Mechanistic Study on Precursor Ions;** [Michal Raab](#); Robert Mistrik; *HighChem, Bratislava, Slovakia*
- TP 526 **Autonomous Orbitrap Platform for Acquisition of MSⁿ Spectral Trees Based on intelligent, Real Time Decision Making Logic;** [Robert Mistrik](#)¹; Jakub Mezey¹; Juraj Lütisan¹; Tim Stratton²; Lukas Najdekr^{2,3}; ¹HighChem, Bratislava, Slovakia; ²Thermo Fisher Scientific, San Jose, CA; ³IMTM, Palacky University, Olomouc, Czech Republic
- TP 527 **Parylene-Matrix Target Chip for Small Molecule Analysis using MALDI-TOF Mass Spectrometry;** [Jo-Il Kim](#); Jong-Min Park; Jae-Chul Pyun; *Yonsei University, Seoul, South Korea*
- TP 528 **"nMS²ⁿ" Approach Aids Characterization of Impurities at Sub-ppm Levels – Capecitabine, an Anti-Cancer Drug;** [Janani Thyagarajan](#); Saravanan Subramanian; Rampriya Uthayakumar; Raman Palvannanathan; Govindarajan Chandramohan; Mohan Kasi; Venkat Manohar; *IICMS, Chennai, India*
- TP 529 **Tandem Mass Spectrometry Characterizes the Related Substances of Second Generation FLT3 Inhibitor Quizartinib, Anti-Cancer Compound for Myeloid Leukemia;** Saravanan Subramanian¹; [Arvind Thyagarajan](#)¹; Rampriya Uthayakumar¹; Raman Palvannanathan¹; Govindarajan Chandramohan¹; Mohan Kasi¹; Venkat Manohar¹; Thaminum Ansari Abubacker²; ¹IICMS, Chennai, INDIA; ²Muthurangam Govt. Arts. College,, Vellore, Tamil Nadu,, India
- TP 530 **Rapid Screening of Adulterated & Counterfeit Products using Bench-Top High Resolution Mass Spectrometer and mzCloud Database Search;** [Philippe Lebel](#)¹; Alexandra Furtos¹; Karen Waldron¹; Kate Comstock²; Tim Stratton²; Maroun El Khoury²; ¹Université de Montréal, Montréal, Qc, Canada; ²Thermo Fisher Scientific, San Jose, CA
- TP 531 **Automated Off-Line SPE LC-MS/MS Method Development using Instrumentation with On-Line SPE Functionality;** [Roy \(TY\) Huang](#); Mike Hastings; Lisa Buchholz; Mingming Ma; *Dow AgroSciences, Indianapolis, IN*
- TP 532 **Degradation Products Analysis of Pantoprazole using High Resolution Mass Spectrometry;** Anoop Kumar¹; [Manoj Pillai](#)¹; Devkant Shandilya²; ¹AB SCIE X, DHR holdings India, Gurgaon, India; ²Bhagwant University, Ajmer, India
- TP 533 **Mass Spectrometry based Combinational Strategy for in vitro and in vivo Metabolite Identification and Confirmation;** [Zheng-Xiang Zhang](#); Tao Bo; *Agilent Technologies (China), Beijing, CHINA*
- TP 534 **Analysis of Additional Impurities in Riboflavin (Vitamin B2) Using a Proposed Alternative USP Method Utilizing LC-MS;** [Carmen T. Santasania](#)¹; Nicolas J. Hauser²; ¹Supelco/Sigma-Aldrich, Bellefonte, PA; ²RTC/Sigma-Aldrich, Laramie, WY
- TP 535 **Identification of Catechol-Group-Contained Compounds by Chloride Anion Approach using APCI/QTOF Mass Spectrometry;** Emily Lichtenberger; [Yufei Chen](#); MIn Li; Nelson Vinuesa; *NC State University, Raleigh, NC*
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- TP 536 **Small-Molecule Spiking for Deuterium Content Reporting in HDX;** [Joey Sheff](#); David Schriemer; *University of Calgary, Calgary, Canada*
- TP 537 **Enzymatic Characterization of Recombinant Nepenthesin II, as a New Tool for Hydrogen/Deuterium Exchange Mass Spectrometry;** [Menglin Yang](#); Martial Rey; David C. Schriemer; *University of Calgary, Calgary, Canada*
- TP 538 **SWATH-based HX-MS² to Investigate Protein Stability of Mitotic Centromere-Associated Kinesin (MCAK) on the Microtubule Lattice;** [Kyle Burns](#); David Schriemer; *University of Calgary, Calgary, Canada*
- TP 539 **Significance of Measured Differences in Comparison Hydrogen Exchange Mass Spectrometry Experiments;** [Rane Harrison](#)¹; Damian Houde²; John Engen¹; ¹Northeastern University, Boston, MA; ²Biogen Idec, Inc., Cambridge, MA
- TP 540 **Combining Ion Mobility Spectrometry with Hydrogen-Deuterium Exchange and Top-Down MS/MS Structure Determination;** [Mahdiar Khakinejad](#); Hossein Maleki; James Arndt; Greg Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- TP 541 **Probing Site-Specific Interactions between Epidermal Growth Factor Receptor and an Adnectin using HDX-ETD MS Approach;** [Jing Fang](#)¹; Stephane Houel¹; Ying-Qing Yu¹; Hui Wei²; Jingjie Mo²; Daniel Cohen²; Dianlin Xie²; Zheng Lin²; Paul Morin²; Michael Doyle²; Adrienne Tymiak²; Weibin Chen¹; Guodong Chen²; ¹Waters Corporation, Milford, MA; ²Bristol-Myers Squibb Company, Princeton, NJ
- TP 542 **Deuteration Effects on the Intrinsic Photophysical Properties of Oxazine Dyes;** Matthew Kusinski; *University of Toronto, Toronto, Canada*
- TP 543 **A two-Site Evaluation of the Repeatability and Precision of an Automated HDX MS Platform;** Alfonso Espada²; David Cummins¹; Scott Novick³; Manuel Molina-Martin²; Devrishi Goswami³; Bruce Pascal³; Ryan Stites¹; Howard Broughton²; [Michael Chalmers](#)¹; Patrick Griffin³; Jeffrey Dodge¹; Juan Espinosa²; ¹Eli Lilly and Company, Indianapolis, IN; ²Lilly S.A., Alcobendas, Spain; ³The Scripps Research Institute, Jupiter, FL

- TP 544 **Subzero Temperature Chromatography Combined with Electron Capture Dissociation for Top-Down Protein Hydrogen Exchange Measurements;** Jingxi Pan¹; Suping Zhang¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²Uvic Dept of Biochemistry and Microbiology, Victoria, Canada
- TP 545 **Purified Protease Type XIII for Enhanced Sequence Coverage in Hydrogen Deuterium Exchange Mass Spectrometry;** Gary Wei; Chengjie Ji; NovaBioAssays, Woburn, MA
- TP 546 **QUDeX-MS: Hydrogen/Deuterium Exchange Calculation for Mass Spectra with Resolved Isotopic Fine Structure;** Joseph Salisbury; Qian Liu; Jeffrey Agar; *Northeastern University, Boston, MA*
- TP 547 **A Novel Approach to Quantitation of Hydrogen Deuterium Exchanged Peptides to Reveal a Distribution of the Exchange at Various Levels;** Yongdong Wang; Ming Gu; Hongliang (Leo) Xu; *Cerno Bioscience, Norwalk, CT*
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- TP 549 **Newly Identified Halogenated Organic Compounds in Technical Pesticide Mixtures and Their Occurrence in Southern California Pacific Dolphins;** Susan A. Mackintosh¹; Eunha Hoh¹; Nellie J. Shaul²; Lihini Aluwihare²; Nathan Dodder³; ¹San Diego State University, San Diego, CA; ²Scripps Institution of Oceanography, La Jolla, CA; ³SCCWRP, Costa Mesa, CA
- TP 550 **Quantitative Determination of Antidepressants and Transformation Products by LC ESI-MS/MS in Terrestrial Environments that Receive Biosolids;** Melissa M. Schultz; Maria Dawaher; Maura Hall; Lydia Niemi; *The College of Wooster, Wooster, OH*
- TP 551 **High Resolution Mass Spectrometry Detection and Identification of Pharmaceutical Transformation Products and Metabolites in Hospital Effluents and Wastewater;** Damià Barceló^{1,2}; Bozo Zonja¹; Noelia Negreira¹; Laura Ferrando - Climent²; Meritxell Gros²; Tina Kosjek³; Sandra Pérez¹; Sara Rodriguez-Mozaz²; Ester Heath^{3,4}; Miren Lopez de Alda¹; ¹Water and Soil Quality Research Group, IDAEA-CSIC, Barcelona, SPAIN; ²Catalan Institute for Water Research (ICRA), Girona, Spain; ³Jozef Stefan Institute, Ljubljana, Slovenia; ⁴Jozef Stefan International Postgraduate School, Ljubljana, Slovenia
- TP 552 **Determination of Emerging Contaminants in Iowa Surface Water at Low PPT Levels Using Direct Injection and SPE LCMSMS;** John Vargo¹; Michael Schueller¹; Mary Skopec²; ¹State Hygienic Laboratory - University of Iowa, Coralville, IA; ²Iowa Geological & Water Survey, Iowa City, IA
- TP 553 **Analysis of Trace Organic Pollutants in Wastewater to Assess Biodegradation using Wrong-way-round Ionization in Liquid Chromatography Tandem Mass Spectrometry;** Lijuan Su¹; Wendell Khunjar²; Diana Aga¹; ¹University at Buffalo, Buffalo, NY; ²Hazen and Sawyer P.C., Fairfax, VA
- TP 554 **Analysis of Veterinary Antimicrobials in Stockpiled Feedlot Manure using LC-ESI/MS/MS;** Srinivas Sura^{1,2}; Dani Degenhardt³; Kerry M. Peru¹; Jonathan Bailey¹; Allan Cessna^{1,2}; Francis Larney⁴; Tim McAllister⁴; Dena McMartin⁵; John Headley¹; ¹Environment Canada, Saskatoon, CANADA; ²Agriculture and Agri-Food Canada, Saskatoon, Canada; ³Alberta Innovates Technology Futures, Edmonton, Canada; ⁴Agriculture and Agri-Food Canada, Lethbridge, Canada; ⁵University of Regina, Regina, Canada
- TP 555 **Investigation of the UV degradation of Diclofenac by means of liquid chromatography and mass spectrometry;** Jörg Roscher; Uwe Karst; *Münster, Germany*
- TP 556 **Rapid and Selective MS/MS Method for Quantification of Light Sensitive Chlortetracycline Drug in Wastewater and Sludge using LDTD Ion Source;** Rama Pulicharla¹; Serge Auger²; Satinder Kaur Brar¹; Patrick Drogui¹; Rao Y. Surampalli³; ¹INRS-ETE, Université du Québec, Québec, Canada; ²Phytronix Technologies, Quebec, CANADA; ³US Environmental Protection Agency, Kansas City, KS
- TP 557 **Identification and Quantitation of Pyrethroids using a GC/QTOF in Negative Chemical Ionization Mode;** Ron Honnold¹; Rafael Acosta²; Matthew Curtis³; ¹Agilent Technologies, Riverside, CA; ²Agilent Technologies, Mexico City, Mexico; ³Agilent Technologies, San Jose, CA
- TP 558 **Sorption Capacities and Interactions of a Mixture of Chemically Diverse Pesticides on Soil using LC-MS/MS;** Heather A. Gamble¹; Donald S. Gamble²; Sha Joshua Ye¹; Ellie Majidi¹; ¹IONICS Mass Spectrometry Group, Inc., Bolton, Canada; ²Department of Chemistry, St. Mary's University, Halifax, Nova Scotia
- TP 560 **Multi-Residue Analysis of Pyrethroids in Soil and Sediment using QuEChERS by LC/MS/MS;** Yuka Fujito¹; Kiyomi Arakawa²; Yoshihiro Hayakawa²; ¹Shimadzu Techno Research, Inc., Kyoto, Japan; ²Shimadzu Corporation, Kyoto, Japan
- TP 561 **Measurement of Multi-Class Herbicides in Dried Environmental Matrices by Paper Spray Ionization Mass Spectrometry;** Steven L. Reeber; Sneha Gadi; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- TP 562 **Application of LC-MS/MS for Monitoring Multiclass Pollutants in Surface and Groundwater;** Zhen Liu¹; Qinghe Wang²; Keyu Zhou²; KeFei Wang²; ¹Southwest Jiaotong University, Chengdu, China; ²Bruker Daltonics, Shanghai, China
- TP 563 **Analysis of Pesticides in Foodstuffs by Gas Chromatography Mass Spectrometry: Evaluation of Various Extraction Procedures;** Mohamed S. Muthanna¹; Esraa Y. Abbas¹; Siham S. Hersi¹; Noor M. Bader¹; Omar Y. Aljarod¹; Abdullah A. Abdulbaker¹; Mohammed F Rakib¹; Shifa M Shaikh¹; Ahmed A. Ramadan¹; Basem Shomar²; Khalid A. Al-Saad¹; ¹Qatar University, Doha, Qatar; ²Qatar Environment and Energy Research Institute, Doha, Qatar
- TP 564 **Evaluation of EN15662:2008 - Determination of Pesticide Residue in Food of Plant Origin, by an Automated QuEChERS Solution;** Tyler Trent¹; James Barlow²; Simon Hird²; Sadat Nawaz²; Tom Hartlein¹; ¹Teledyne Tekmar, Mason, Ohio; ²The Food and Environment Research Agency, York, UK
- TP 565 **Rapid Identification of Environmental Contaminants using High Resolution LC/MS/MS in Combination with Library Search;** Michael P. Schluesener¹; Jianru Stahl-Zeng²; Thomas A. Ternes¹; Detlev Schleuder²; ¹Federal Institute of Hydrology, Department Aquatic, Koblenz, Germany; ²AB Sciex, Darmstadt, Germany
- TP 566 **Chiral Separation of Three β -blocking Pharmaceuticals and a Major Metabolite using SFC-MS;** Alfred Swan¹; Mikael Hedeland²; Torbjörn Arvidsson¹; Curt Pettersson¹; ¹Uppsala University, Uppsala, Sweden; ²Nat'l Veterinary Institute, Uppsala, Sweden
- TP 567 **Multiple Elemental Compound Identification by GCxGC-ICP-MS;** Kevin Huncik; *National Institute of Standards and Technology, Charleston, SC*
- TP 568 **An Enhanced Method for Extraction and Quantification of Highly Lipophilic Pyrethroid Pesticides from Adipose Tissue;** Holly C. Young; Darren R. Gullick; Andrew Popovici;

- James V. Bruckner; Brian S. Cummings; Michael G. Bartlett; *University of Georgia, Athens, GA*
- TP 569 **Unusual Fragmentation of N-Perfluoroacetyl(cycloalkyl)amines; Kirill V. Tretyakov;** Nino G. Todua; Anzor I. Mikaia; *National Institute of Standards and Technology, Gaithersburg, MD*
- TP 570 **Detection of Herbicidal Glyphosate from Environmental Matrices using Matrix-Assisted Inlet Ionization Mass Spectrometry (MAIL-MS); Julie Mercadante;** Sarah Saylor; Catherine Bentzley; *University of the Sciences, Philadelphia, PA*
- TP 571 **Automated Detection of Trace Level Basic and Acidic Pesticides and Herbicides in Drinking Water by Online SPE LC/MS; Edgar Naegele²;** Dorothy Yang¹; ¹ Santa Clara, CA; ²Agilent Technologies, Waldbronn, N/A
- TP 572 **Accurate LCMS Spectral Assignments and Quantification: Methodology and Tools for Pesticides Analyses; Tukiet T. Lam¹;** Ming Gu²; Jean Kanyo¹; Yongdong Wang³; ¹Yale University, New Haven, CT; ²Cerno Bioscience, Yardley, PA; ³Cerno Bioscience, Norwalk, CT
- TP 573 **Glyphosate and AMPA Analysis in Drinking Water Using Two-Dimensional Liquid Chromatography Mass Spectrometry (2D LC/MS/MS);** Claude Mallet; *Waters Corporation, Milford, MA*
- TP 574 **Quantitative Performance of the Q-Exactive High-Resolution Accurate-Mass (HR/AM) Spectrometer for the Analysis of Tetracyclines in a Complex Environmental Matrix; Morgan Sollicie;** Audrey Roy-Lachapelle; *Université de Montréal, Montréal, Canada*
- TP 575 **Oxidative Removal of Selected PPCPs and Identification of Oxidative Degradates of PPCPs in Drinking Water Using LC-MS/MS; Yinfa Ma¹;** RuiPu Mu¹; Honglan Shi¹; Craig Adams²; Todd Eichholz³; ¹Missouri S&T, Rolla, MO; ²Utah State University, Logan, UT; ³Missouri Department of Natural Resources, Jefferson City, MO
- TP 576 **Pre-concentration, Separation and high-Resolution Tandem Mass Spectrometry Identification of Intermediate Products of Sulfamethazine Antibiotic Formed by Photochemical Degradation in Water;** Tanare Ferreira; Júlia Martins; Amanda Imamura; Leonardo Medinilha; Fernando Lanças; *Alvaro Santos-Neto; University of São Paulo, São Carlos, Brazil*
- TP 577 **High Resolution Mass Spectrometry Based Metabolomics: a New Tool to Detect and Characterize Emerging Pollutants in Water and Food Matrices; Jerome Cotton^{1,2};** Fanny Leroux²; Simon Broudin²; Bruno Corman²; Jean-Claude Tabet³; Celine Ducruix²; Christophe Junot¹; ¹CEA, iBiTec-S/SPI/LEMM, Gif-Sur-Yvette, FRANCE; ²Profilomic, Boulogne-Billancourt, France; ³UPMC - LCSOB, Paris, France
- TP 578 **Quantitative and Semi-Quantitative Determination of PPCPs and By-products in Wastewater Treatment Plants Samples Using UHPLC-Orbitrap MS and Data Mining Technologies; Paul Yang³;** Tung-Vi Nguyen¹; Ramin Farnood¹; Dipankar Ghosh⁴; Jonathan Beck⁴; Maciej Bromirski²; Charles Yang⁴; ¹University of Toronto, Toronto, Canada; ²Thermo Fisher Scientific GmbH, Bremen, N/A; ³Ontario Ministry of the Environment, Etobicoke, Canada; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 579 **EPA Draft Method 543 Quantitation of Organic Pesticides in Drinking Water Using Online Pre-concentration/Solid Phase Extraction and Tandem Mass Spectrometry; Jonathan Beck;** Charles Yang; *Thermo Fisher Scientific, San Jose, CA*
- TP 580 **Semi Real Time Screening of PPCP and Pesticide by Field Type Water Sampler with Online SPE-HRAM; Jaewon Choi¹;** Charles T. Yang²; Dipankar Ghosh²; ¹Kwater, Daejeon, South Korea; ²Thermo Fisher Scientific, San Jose, CA
- TP 581 **Systematic Elucidation of Matrix Effects in liquid Chromatography Hyphenated to Mass Spectrometry; Norbert Wenkel¹;** Thorsten Teutenberg²; Jochen Tuerk²; Christoph Portner²; Claudia Vom Eyser²; Sandy-Dominic Freihoff¹; ¹Axel Semrau GmbH, Sprockhovel, Germany; ²Institut für Energie- und Umwelttechnik e.V., Duisburg, Germany
- TP 582 **Gain Productivity and Increase Data Quality with the GC/MS/MS Pesticide Analyzer; Jessica Westland;** Bruce Quimby; Kai Meng; *Agilent Technologies, Wilmington, Delaware*
- TP 583 **Fast and Highly Sensitive Analysis of Multiple Drugs in Ground-, Surface- and Wastewater; Klaus Bollig¹;** Sven Vedder²; Anja Grüning²; ¹Shimadzu Deutschland GmbH, Duisburg, Germany; ²Shimadzu Europe GmbH, Duisburg, Germany
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- TP 584 **Crude Oil Transformation during Rock Migration via FTICR-MS: From Source Rock to Reservoir; Marcos Pudenzi¹;** Eduardo Schmidt¹; Jose Jara¹; Heliara Nascimento¹; Elias Tessaro¹; Vanessa Santos¹; Pedro Henrique Vendramini¹; Rosana Pereira²; Wagner Bastos²; Erica Morais²; Alessandro Batezelli¹; Marcos Eberlin¹; ¹UNICAMP, Campinas, BRASIL; ²Petrobras, Rio de Janeiro, Brasil
- TP 585 **Structural Study of Asphaltenes by Laser Desorption Ionization Mass Spectrometry Coupled to Traveling Wave Ion Mobility; Hector Koolen;** Alexandre Gomes; Lyzette Moura; Franca Marcano; Felipe Cardoso; Paulo Rosa; Fabio Gozzo; *UNICAMP, Campinas, Brazil*
- TP 586 **Petroleomics by TWIM-MS: Print Screen of Addictives used in Crude Oil Industry; Jandyson Machado Santos¹;** Heliara D. L. Nascimento¹; Elias Tessaro¹; Vanessa Gonçalves Santos¹; Marcos A. Pudenzi¹; Eduardo M. Schmidt¹; Renan de S. Galaverna¹; Rosana C. L. Pereira²; Wagner L. Bastos²; Erica T. de Moraes²; Gleber Tacio Teixeira²; Maira Fasciotti³; Alberto Wisniewski Junior⁴; Marcos N. Eberlin¹; ¹Institute of Chemistry - UNICAMP, Campinas, BRAZIL; ²PETROBRAS, Rio de Janeiro, Brazil; ³INMETRO, Rio de Janeiro, Brazil; ⁴Chemistry Department - UFS, São Cristóvão, Brazil
- TP 587 **Study of Asphaltene Aggregation by MALDI-TOF-MS; Martha L. Chacón-Patiño¹;** Andrea Gómez-Escudero²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Instituto Colombiano del Petróleo, Piedecuesta, Colombia
- TP 588 **Phenylenevinylene Derivatives as MALDI Matrices for Electron Transfer Ionization of Asphaltene Model Compounds; Laura J. Castellanos-García¹;** Martha L. Chacón-Patiño¹; Brian Castro²; Alexander Scherer³; Xiaoli Tan⁴; Rik R. Tykwinski³; Murray R. Gray⁴; César A. Sierra-Ávila²; Cristian Blanco-Tirado¹; *Marianny Y. Combariza¹;* ¹Escuela de Química, Univ Industrial de Santander, Bucaramanga, Colombia; ²Departamento de Química, Univ Nacional de Colombia, Bogotá, Colombia; ³University of Erlangen-Nürnberg, Erlangen, Germany; ⁴Dept of Chem and Mat Eng, University of Alberta, Edmonton, Canada
- TP 589 **Elucidation of Structural Information for Asphaltenes via Collision-Activated Dissociation of Their Molecular Ions in MSⁿ Experiments: A Model Compound Study;**

- Chunfen Jin¹; Tiffany Jarrell¹; James Riedeman¹; Benjamin Owen¹; Xiaoli Tan³; Alexander Scherer²; Rik Tykewski²; Murray Gray³; Peter Slater⁴; Hilikka Kenttämä¹; ¹Purdue University, West Lafayette, IN; ²University of Erlangen-Nuremberg, Erlangen, Germany; ³University of Alberta, Edmonton, Alberta; ⁴ConocoPhillips, Houston, TX
- TP 590 **Distillate Fraction Composition Estimation Using Crude Oil Petroleomics**; Fan Huang; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- TP 591 **Analysis of Pre-Separated Crude Oil Using an Orbitrap**; Matthew Hurt; Michael Cheng; Chevron, Richmond, CA
- TP 592 **Electrospray Ionization for Determination of Non-Polar Polyaromatic Hydrocarbons and Polyaromatic Heterocycles in Crude Oil Asphaltenes**; Lilla Molnár; Guricza; Wolfgang Schrader; Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany
- TP 593 **High-Resolution Online LC/MS for Characterizing Crude Oils – Grinding the Data**; Alessandro Vetere; Wolfgang Schrader; Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany
- TP 594 **Evaluation of Polar Composition Changes in Diesel Fuels by FT-ICR MS after Stability Test**; Rosana C. L. Pereira¹; Helineia O. Gomes¹; Manoel J.R. Guimarães Neto¹; Felipe C. Gouveia¹; Boniek G. Vaz²; ¹Petrobras/CENPES, Rio de Janeiro, Brazil; ²UFG, Goiânia, Brazil
- TP 595 **Dynamic Range Enhancement Stitching of Multiple Ultrahigh Resolution FT-ICR Mass Spectral Segments**; Logan C. Krajewski¹; Yuri E. Corilo^{2,3}; Ryan P. Rodgers^{2,3}; Alan G. Marshall^{1,3}; ¹FSU Department of Chemistry and Biochemistry, Tallahassee, FL; ²Florida State University Future Fuels Institute, Tallahassee, FL; ³Ion Cyclotron Resonance Prog, Tallahassee, FL
- TP 596 **Targeted Ionization of Oxygen-Containing Compounds in Petroleum Crude Oil by Lithium Cationization**; Electrospray Ionization FT-ICR Mass Spectrometry; Rebecca Beasley¹; Vladislav Lobodin^{2,3}; Alan Marshall^{1,3}; Ryan Rodgers^{1,3}; ¹Florida State University, Tallahassee, FL; ²Future Fuels Institute, Tallahassee, FL; ³National High Magnetic Field Laboratory, Tallahassee, FL
- TP 597 **FT-ICR MS Imaging of Thin Layer Chromatograms of Crude Oil, Field Deposit, and Weathered Oil**; Donald F. Smith^{1,4}; Amy M. McKenna¹; Yuri E. Corilo^{1,2}; Ryan P. Rodgers^{1,3}; Alan G. Marshall^{1,3}; Ron M.A. Heeren⁴; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Florida State University, Tallahassee, FL; ³Department of Chemistry and Biochemistry, FSU, Tallahassee, FL; ⁴FOM Institute AMOLF, Amsterdam, The Netherlands
- TP 598 **Modifications to a Novel Method for the Isolation of Interfacial Material from Athabasca Bitumen: Characterization by FT-ICR Mass Spectrometry**; Amy C. Clingenpeel¹; Jacqueline M. Jarvis²; Winston K. Robbins³; Alan G. Marshall^{1,2}; Ryan P. Rodgers^{1,2}; ¹Florida State University, Tallahassee, FL; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Future Fuels Institute, Tallahassee, FL
- TP 599 **Structural Investigation of Interfacially Active Compounds from Petroleum Crude Oil by FT-ICR Mass Spectrometry**; Jacqueline M. Jarvis¹; Benjamin J. Bythell²; Chad R. Weisbrod¹; Alan G. Marshall^{1,3}; Ryan P. Rodgers^{1,3}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²University of Missouri-St. Louis, St. Louis, MO; ³Florida State University, Tallahassee, FL
- TP 600 **Characterization, Chromatographic Enrichment, and Trace Metal Analysis of Nickel and Vanadyl Porphyrins from Weathered Natural Seeps by FT-ICR and ICP-MS**; Jonathan Putman¹; Amy M. McKenna¹; Jeffrey T. Williams¹; Ryan P. Rodgers^{1,2}; Alan G. Marshall^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Department of Chemistry and Biochemistry, Tallahassee, FL
- TP 601 **Determination of Isomers in Petroleum by Ion Mobility Mass Spectrometry**; Priscila M. Lalli¹; Steven M. Rowland¹; Yuri E. Corilo^{1,2}; Ryan P. Rodgers^{1,2}; Alan G. Marshall^{1,3}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University Future Fuels Institute, Tallahassee, FL; ³Florida State University, Department of Chemistry, Tallahassee, FL
- TP 602 **Petroleomics: Progress Toward its Full Predictive Power via a Comprehensive Model of the Petroleum Continuum**; Yuri E. Corilo^{1,2}; Priscila M. Lalli¹; Ryan P. Rodgers^{1,3}; Alan G. Marshall^{1,3}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Florida State University, Tallahassee, FL; ³Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- TP 603 **High Performance Time-of-Flight Mass Spectrometry for Comprehensive Petroleum Analysis**; Clécio Klitzke; David Alonso; Joe Binkley; Jeffrey Patrick; LECO Corporation, St. Joseph, Michigan
- TP 604 **Identification of Organic Compounds in Crude Oils without Catalyst Treatment by Comprehensive Two-Dimensional GC/HRTOFMS**; Morio Ueda¹; Koji Okuda²; Jun Onodera²; Akihiko Kusai²; Jonathon Bunn³; Yoshika Tennichi¹; Hidehisa Kawamura¹; Joo-il Park⁴; Seongho YOON⁴; Isao Mochida⁴; ¹Kyushu Environmental Evaluation Association, Fukuoka, Japan; ²JEOL Ltd., Tokyo, Japan; ³JEOL USA, Inc., MA; ⁴Kyushu University, Fukuoka, Japan
- TP 605 **Genetic Link between Fatty Acids and Hydrocarbons produced During Artificial Maturation of a Type I Kerogen using ESI-FT-ICR-MS and GCxGC-MS**; Albert Kamga¹; Françoise Behar²; Patrick G. Hatcher¹; ¹ODU Research Foundation, Norfolk, VA; ²TOTAL SA, Paris, France
- TP 606 **Pressurized Heating for the Rapid Preparation/ Extraction of Coal Samples for Broad Spectrum GC-MS Analysis**; Franco Basile¹; Rajendra Mahat¹; Wesley Rodgers²; ¹University of Wyoming, Laramie, WY; ²JR Simplot Co, Boise, ID
- TP 607 **Ultra-Fast Profiling of C20-C60 Alkanes in Waxed Samples using LDTD-MS/MS**; Serge Auger; Gregory Blachon; Pierre Picard; Phytronix Technologies, Quebec, Canada
- TP 608 **Pulsed Flow Modulation GCxGC-MS with Cold EI**; Uri Keshet¹; Tal Alon^{1,2}; Alexander Fialkov¹; Aviv Amirav^{1,2}; ¹Tel-Aviv University, Tel-Aviv, ISRAEL; ²Aviv Analytical LTD, Tel Aviv, Israel
- TP 609 **Correlation Studies between Chemical Properties of Crude Oils and Mass Spectrometric Analysis on the Molecular Level using LDI and APPI**; Matthias Witt; Gökhan Baykut; Bruker Daltonik GmbH, Bremen, Germany
- TP 610 **Molecular Level Analysis of TLC Fractions of Crude Oil by LDI FT-ICR Mass Spectrometry**; Matthias Witt¹; Mike Easterling²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA
- TP 611 **Drug Metabolism: Qualitative Analysis, 611 - 636**
- Rapid Mass Spectrometric Detection of Drug Metabolites Generated in a Microfluidic Electrochemical Cell**; Lars Büter¹; Floris T.G. van den Brink²; Mathieu Odijk²; Wouter Olthuis²; Albert van den Berg²; Uwe Karst¹; ¹University of Münster, Münster, Germany; ²University of Twente, Enschede, The Netherlands

- TP 612 **Simulation of Metabolic Processes of Polycyclic Aromatic Hydrocarbons using Electrochemistry/Mass Spectrometry**; [Tina Wigger](#)^{1,2}; [Lars Bütter](#)^{1,2}; [Uwe Karst](#)¹; ¹University of Münster, Münster, Germany; ²NRW Graduate School of Chemistry, Münster, Germany
- TP 613 **MsXelerator: A Software Platform for Drug Metabolite Detection and Identification using High-Resolution Mass Spectrometry and Post-Acquisition Data Mining**; [Marco Ruijken](#); *MsMatrix, Maarssen, Netherlands*
- TP 614 **Application of LC-MSⁿ and NMR Techniques in Identification of *In Vitro* Metabolites**; [Regina V. Oliveira](#)¹; [Josiane de O. Cardoso](#)¹; [Bianca F. da Silva](#)¹; [Tiago Venâncio](#)¹; [Rosângela G. Peccinini](#)²; [Ivan R. Pitta](#)³; [Maria do Carmo A. de Lima](#)³; ¹Chemistry Department, Federal University of São Carlos, São Carlos, SP, Brazil; ²College of Pharmaceutical Sciences, State University of São Paulo, Araraquara, SP, Brazil; ³Group of Research in Therapeutic Innovation, Federal University of Pernambuco, Recife, PE, Brazil
- TP 615 **Antitumor Steroidal Lactone Withaferin A in Human Breast Cancer Cells Is Covalently Bound to Cysteine-303 of β -Tubulin**; [Guy Uechi](#); [Marie Lue Antony](#); [Eun-Ryeong Hahm](#); [Shivendra Singh](#); [Nathan Yates](#); *University of Pittsburgh, Pittsburgh, PA*
- TP 616 **Metabolite Profiling Using Human Hepatocyte Co-cultures and UHPLC-Q-TOF-MS with Data Independent MS/MS**; [Ronghua Wang](#)¹; [Ragu Ramanathan](#)¹; [Cornelia Smith](#)²; [Caroline Lee](#)²; [Helen Shen](#)¹; [Zamas Lam](#)¹; ¹QPS, LLC, Newark, DE; ²QPS Hepatic Biosciences, Research Triangle Park, NC
- TP 618 **Characterisation of Metabolites by Utilising Collision Cross Section Measurements in Conjunction with an Integrated Microfluidic Device**; [Richard T. Gallagher](#)¹; [Christine Pattison](#)¹; [Kathryn Pickup](#)¹; [Kristin Samuelsson](#)¹; [Mike McCullagh](#)²; [David S Douce](#)²; ¹AstraZeneca, Macclesfield, UK; ²Waters (MS Technologies), Manchester, UK
- TP 619 **Identification of the Microbial Fermentation Products for Curcumin using Metabolite ID Workflow Based on High Resolution Mass Spectrometry**; [Dezhao Lu](#)¹; [Xiaoyan Xu](#)²; [Ting Liu](#)²; [Kerong Zhang](#)²; [Huafen Liu](#)²; [Xingde Wo](#)¹; ¹College of Life Science, Zhejiang Chinese Medical University, Hangzhou, Zhejiang Province, China; ²AB SCIEX Asia Pacific Application Support Center, Shanghai, China
- TP 620 **Are Low Flow Mass Spectrometry Techniques Reliable Enough to be used for Metabolite Estimation from Human Samples without Standards?**; [Jill L. Pirhalla](#); *GlaxoSmithKline, King Of Prussia, PA*
- TP 621 **Identification of Rilpivirine Metabolites in Human Liver Microsomes and Characterization of Cytochrome P450 Enzymes Involved in the Biotransformation by LC-MS/MS**; [Josiane de Oliveira Cardoso](#)^{1,2}; [Jessica Bo Li Lu](#)¹; [Regina Vincenzi Oliveira](#)²; [Zeruesenay Desta](#)¹; ¹Division of Clinical Pharmacology, Indiana University School of Medicine, Indianapolis, IN; ²Chemistry Department, Federal University of São Carlos, São Carlos, SP, Brazil
- TP 622 **Electrochemistry/MS – a Powerful Tool in Drug Metabolism**; [Martin Eysberg](#); [Agnieszka Kraj](#); [Hendrik-Jan Brouwer](#); [Nico Reinhoud](#); [Jean-Pierre Chervet](#); *Antec (USA), Boston, MA*
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- TP 624 **Investigation of d6-Bisphenol A Diconjugates in Humans Following Oral Administration of d6-BPA on a Cookie**; [Mona I. Churchwell](#); [Nathan C. Twaddle](#); [Daniel R. Doerge](#); *NCTR/FDA, Jefferson, AR*
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- TP 626 **Soft-Spot Identification for Drug Discovery: Utilizing Sciex AB 5600 Information Dependent Acquisition Scanning, MassMetasite Software and WebMetabase Browser**; [Kerry Fillgrove](#)¹; [Diane Grotz](#)²; [Somang Kim](#)¹; [Ian Knemeyer](#)³; [Kevin Bateman](#)¹; ¹Merck Research Labs, West Point, PA; ²Merck Research Labs, Kenilworth, NJ; ³Merck Research Labs, Boston, MA
- TP 627 **Exploiting Variable Swath Techniques to Maximize the Quality of MS/MS Spectra for Metabolite Identification Studies**; [Richard Schneider](#)¹; [Veronica Zelesky](#)²; [Eva Duchoslav](#)³; ¹Pfizer Global R&D, Groton, CT; ²Pfizer Inc., Groton, CT; ³AB Sciex, Concord, ON
- TP 628 **High Resolution Mass Spectrometric Investigation of the *in vivo* Metabolism of Selective Androgen Receptor Modulators (SARMs) in the Horse**; [Mikael Hedeland](#)⁴; [Annelie Hansson](#)¹; [Axel Rydevik](#)¹; [Oliver Krug](#)²; [Mario Thevis](#)²; [Ulf Bondesson](#)⁴; [Heather Knych](#)³; [Scott Stanley](#)³; ¹Uppsala University, Uppsala, Sweden; ²German Sport University, Cologne, Germany; ³University of California - Davis, Davis, CA; ⁴National Veterinary Institute, Uppsala, Sweden
- TP 629 **Utilizing Ion Mobility Drift Times to Correlate and Track Metabolites across Changing Chromatographic Methods and Modes including SFC and UHPLC**; [Hernando Olivos](#)¹; [Adam Ladak](#)¹; [Andrew Baker](#)³; [Steven Lai](#)¹; [Yun Alelyunas](#)²; [Paul Rainville](#)²; [Mark Wrona](#)²; ¹Waters, Beverly, MA; ²Waters, Milford, MA; ³Waters, Pleasanton, CA
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- TP 633 ***In vitro* Species Comparison using Long-term Hepatocyte Co-Culture Models and Highly Sensitive UHPLC-Q-TOF-MS with SWATH Analysis**; [Jian Yu](#)¹; [Ragu Ramanathan](#)¹; [Cornelia Smith](#)²; [Caroline Lee](#)²; [Helen Shen](#)¹; [Zamas Lam](#)¹; ¹QPS, LLC, Newark, DE; ²QPS Hepatic Biosciences, Research Triangle Park, NC
- TP 634 **Metabolic Stability Assay Using Human Hepatocyte Co-cultures and Integrated Qualitative/Quantitative High Resolution Mass Spectrometry**; [Alex Zang](#)¹; [Ragu Ramanathan](#)¹; [Cornelia Smith](#)²; [Caroline Lee](#)²; [Helen Shen](#)¹; [Zamas Lam](#)¹; ¹QPS, LLC, Newark, DE; ²QPS Hepatic Biosciences, Research Triangle Park, NC
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- TP 638 **Development of a Biological Internal Reference for Full Scan LC-MS Metabolomics Applied to the Cellular Stress Response;** Amy Caudy; Olga Zaslaver; Julia Hanchard; Christopher Go; Ying Zhang; Adam Rosebrock; *University of Toronto, Toronto, Canada*
- TP 639 **Untargeted Metabolomic Analysis for the Evaluation of Stress Effects on Model Organisms;** Joaquim Jaumot¹; Meritxell Navarro¹; Elena Ortiz¹; Alejandro García-Reiriz^{1, 2}; Marta Casado¹; Benjamín Piña¹; Romà Tauler¹; *1IDAEA-CSIC, Barcelona, Spain; 2QUIR-CONICET, Rosario, Argentina*
- TP 640 **Single-cell Metabolomics and Proteomics by Capillary Electrophoresis ESI MS;** Peter Nemes¹; Jordan T. Aerts²; Rosemary M. Onjiko¹; Stanislav S. Rubakhin²; Jonathan V. Sweedler²; *1George Washington University, Washington, DC; 2University of Illinois--Urbana-Champaign, Urbana, IL*
- TP 641 **Direct Tissue Spray Ionization of Living Plants by Mass Spectrometry for Metabolomics;** Dana M. Freund; Amanda C. Martin; Jerry D. Cohen; Adrian D. Hegeman; *University of Minnesota, St. Paul, Minnesota*
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- TP 643 **Metabolomics Profiling using Atmospheric Pressure Gas Chromatography-MS;** Vladimir Shulaev²; Ghaste Manoj^{2, 3}; Steven Lai¹; Carolina Salazar²; Nobuhiro Suzuki²; Janna Crossley²; Ron Mittler²; James Langridge¹; Giuseppe Astarita¹; Fulvio Mattivi³; *1Waters Corporation, Milford, MA; 2University of North Texas, Denton, TX; 3Fondazione Edmund Mach, San Michele all'Adige, Italy*
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- TP 645 **Comparative Metabolomic Studies on Two Chinese Podophyllum Plants;** Xiaoming Jiang¹; Mingquan Guo^{1, 2}; *1Wuhan Botany Garden, Chinese Academy of Sciences, Wuhan, China; 2University of Southern California, Alhambra, CA*
- TP 646 **Profiling of Specialized Metabolites that Accumulate in Trichomes of *Petunia* species;** Xiaoxiao Liu¹; Cornelius S. Barry³; A. Daniel Jones^{1, 2}; *1Department of Chemistry, Michigan State University, East Lansing, MI; 2Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; 3Department of Horticulture, Michigan State University, East Lansing, MI*
- TP 647 **Comprehensive Untargeted Metabolite Profiling of Alangifolium Salvifolium Bark using LCMS and GCMS Techniques;** Siddaiah Chandranayak¹; Harischandra Sripathi Prakash¹; Syed Salman Lateef²; Saligrama Adavigowda Deepak²; *1Department of Studies in Applied Botany/Biotechnol, Mysore, Karnataka, India; 2Agilent Technologies, Bangalore, INDIA*
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- TP 656 **Hemorrhagic Shock "fingerprint" Based on Global Metabolite Profiling of Porcine Urine Sample;** Monika Tokmina-Lukaszewska¹; Navid Movahed¹; Elizabeth Lusczek²; Kristine Mulier²; Greg Beilman²; Brian Bothner¹; *1Department of Chemistry & Biochemistry, Bozeman, MT; 2Department of Surgery, University of Minnesota, Minneapolis, MN*
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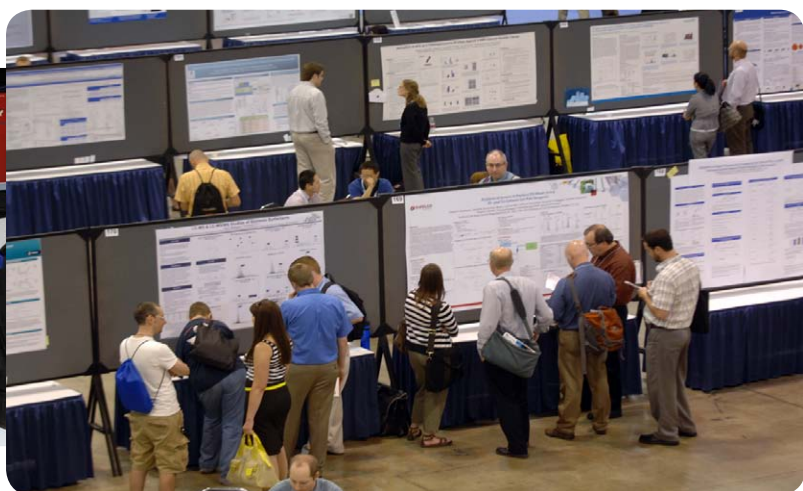
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- TP 679 **Combination of Different Extraction, Separation and Mass-Spectrometric Approaches for Identification of Complex Mixtures of Volatile Compounds Emanated from Tropical Flowers**; [Elena Stashenko](#); Silvia Cardenas; Corina Bernal; Jairo Rene Martinez; *Universidad Industrial de Santander, Bucaramanga, Colombia*
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- TP 684 **Dwell Time, a Critical Factor on Precision in N-in-One Assays Utilizing UPLC-MS/MS**; [Lan Li](#); Tracey Wilson; Yuan-Shek Chen; Luca Matassa; *QPS, LLC, Newark, DE*

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- TP 686 **Cross-Species Quantification of Snake Venoms using iTRAQ;** Erika Velásquez¹; Rafael D Melani¹; Paulo Costa Carvalho²; Diogo B Lima²; Magno Junqueira¹; Fabio CS Nogueira¹; Gilberto Domont¹; ¹Univ Federal Do Rio De Janeiro, Rio De Janeiro, Brazil; ²Carlos Chagas Institute, Curitiba, Pr
- TP 687 **Improved Identification and Extended Quantitative Mass Range of Peptide Tagged TMT by Combined N-Terminal Enzyme and Triple-Stage Mass Spectrometry;** Ya-Ping Lin; Chein-Hung Chen; Jung-Lee Lin; Chung-Hsuan Chen; *Genomics Research Center, Academia sinica, Taipei, Taiwan*
- TP 688 **Application of Multistage Tandem Mass Spectrometry for Quantification of Endogenous Metabolites In Lung Tissue;** Keely Pierzchalski¹; Jace W. Jones¹; Catherine Booth²; Gregory Tudor²; Alexander Bennett³; Ann Farese³; Thomas MacVittie³; Pu-Ting Xu³; Isabel Jackson³; Zeljko Vujaskovic³; Maureen Kane¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD; ²Episteme Ltd, Manchester, UK; ³University of Maryland, School of Medicine, Baltimore, MD
- TP 689 **Stable Isotope Labeled Internal Standards in Quantification of Biomolecules using LC MS/MS;** Meiyao Wang; Illarion Turko; *NIST, IBBR, Rockville, MD*
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- TP 692 **Understanding Protein Expression Levels and Quantitation in Single Cell Analyses Using ICP-QQQ;** Jonathan Wanagat¹; Amir Liba²; ¹UCLA, Dept. of Medicine, Los Angeles, CA; ²Agilent Tech., Wilmington, DE
- TP 693 **Achieving Maximal Sensitivity Gain When Scaling a Protein Immunocapture Assay from Traditional to Low Micro-Flow LC-MS/MS;** Eugene F. Ciccimaro¹; Bogdan Sleczyka¹; John T. Mehl¹; Lorell Disenza¹; Asoka Ranasinghe¹; Celia D'Arienzo¹; Jim Murphy³; Brad Coopersmith²; Paul Rainville³; Catalin Doneanu³; Timothy Olah¹; ¹Bristol-Myers Squibb, Princeton, NJ; ²Waters, Richboro, PA; ³Waters, Milford, MA
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- TP 710 **Ion Enhancement and MS/MS for Analysis of Organics in Complex Mars Analog Matrices with the MOMA Ion Trap Mass Spectrometer;** Ryan M. Danell¹; Friso H.W. van Amerom²; Veronica Pinnick³; Xiang Li³; Stephanie Getty³; Ricardo Arevalo³; William Brinckerhoff³; Paul Mahaffy³; ¹Danell Consulting, Inc., Winterville, NC; ²Mini-Mass Consulting, Inc., Hyattsville, MD; ³NASA GSFC, Greenbelt, MD
- TP 711 **High Speed and Accurate Pressure Measurement with a micro Pirani Pressure Gauge for Pressures from 100 mTorr to sub 1mTorr. ;** Adrian Southard¹; Tomoko Adachi²; Ricardo Arevalo³; Gary Brown³; Christopher Johnson³; Zachary Gonnsen⁴; Stephen Meyer³; William Brinckerhoff³; Paul Mahaffy³; ¹University Space Research Agency, Greenbelt, Maryland; ²Catholic University, Washington, DC; ³NASA GSFC, Greenbelt, MD; ⁴Microtell LLC, Greenbelt, MD - Maryland
- TP 712 **Micro Mass Analyzer for the Investigation of Cometary Bodies;** Ashish Chaudhary¹; Tim Short¹; Michelle Cardenas¹; Emily Barrentine²; Danny Glavin²; Paul Mahaffy²; William Brinckerhoff²; Yun Zheng²; Friso H.W. Van Amerom¹; ¹SRI International, St. Petersburg, FL; ²NASA GSFC, Greenbelt, MD
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- TP 714 **Development of a Hybrid Ion Mobility Spectrometry/ Time-of-Flight Mass Spectrometer with Printed Circuit Board Technology;** Ian K. Webb; Tsung-Chi Chen; Xinyu Zhang; Sandilya V. B. Garimella; Randolph V. Norheim; Gordon A. Anderson; Yehia M. Ibrahim; Keqi Tang; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 715 **Improving Mass Spectrometric Sensitivity and Ionization Efficiency Using a nanoESI Emitter Array at Subambient Pressures;** Jonathan T. Cox; Ioan Marginean; Ryan Kelly; Richard D. Smith; Keqi Tang; *Pacific Northwest National Laboratory, Richland, WA*
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- TP 717 **Fundamental Aspects of Ion Confinement in SLIM Devices;** Aleksey V. Tolmachev; Xinyu Zhang; Sandilya V.B. Garimella; Ian K. Webb; Yehia M. Ibrahim; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 718 **A Novel Linear Ion Trap Mass Analyzer built with Triangular Electrodes;** Chuan-fan Ding; Yu Xiao; *Fudan University, Shanghai, China*
- TP 719 **Accelerating 2D FT-ICR by non-Uniform Sampling and Maximum Entropy Reconstruction for Increased Resolution and/or Decreased Acquisition Time;** Fabrice Bray¹; Lionel Chiron²; Marie-Aude Coutouly²; Caroline Tokarski¹; Marc-André Delsuc³; Christian Rolando¹; ¹Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France; ²NMRTEC, Illkirch-Graffenstaden, France; ³IGBMC, Illkirch-Graffenstaden, France
- TP 720 **Toward Determination of Ion Collision Cross Sections for Biomolecules within FT-ICR Cells;** Lu Mao¹; Yu Chen¹; Yu Chen²; Nathan K. Kaiser²; Alan G. Marshall^{2, 3}; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, CHINA; ²ICR Program, National High Magnetic Field Lab, Tallahassee, FL; ³Department of Chemistry & Biochemistry, FSU, Tallahassee, FL
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- TP 723 **Design and Utility of a Multi-Pass Cyclic Ion Mobility Separator;** [Kevin Giles](#); Jason L Wildgoose; Steven Pringle; John Garside; Peter Carney; Peter Nixon; David Langridge; *Waters Corporation, Wilmslow, UK*
- TP 724 **The Extraction of Maximum Information from Individual Ion Arrivals and Its Application to Extending the Dynamic Range of IMS-ooToF-MS Data;** [Martin Green](#); Garry Scott; Darrell Williams; Tony Gilbert; Keith Richardson; Martin Palmer; Nick Tomczyk; *Waters Corporation, Manchester, UK*
- Instrumentation: New Developments in Ionization and Sampling, 725 - 745**
- TP 725 **Alternating Current Corona Discharge APCI Ion Source for the Detection of Explosives;** [Dilshadbek Usmanov](#)^{1,2}; Lee Chuin Chen¹; Kenzo Hiraoka¹; ¹*University of Yamanashi, Kofu, Japan*; ²*Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*
- TP 726 **Analysis of Non-Volatile Samples by Flash Desorption/Mass Spectrometry;** [Kenzo Hiraoka](#)¹; Dilshadbek Usmanov^{1,2}; Satoshi Ninomiya¹; ¹*University of Yamanashi, Kofu, Japan*; ²*Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*
- TP 727 **Applications of Super-Atmospheric Pressure ESI in Superheated ESI-MS and Nano-ESI using Disposable Pipet Tip;** [Lee Chuin Chen](#); Md. Matiur Rahman; Kenzo Hiraoka; *University of Yamanashi, Kofu, Japan*
- TP 728 **Plasma Induced Secondary Ionization - Ion Mobility Spectrometry (PISI-IMS) for Real Time Drug Quality Assessment;** [Prabha Dwivedi](#)¹; Paula Holmes²; Adam Kaylor¹; Facundo M. Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Photonis USA Inc., Sturbridge, MA*
- TP 729 **Microplasma Ion Source for Rapid Air/Water Volatile Organic Contaminant Analysis on board the International Space Station;** [Rosana M. Alberici](#)²; Joel D. Keelor¹; Josh M. Symonds¹; Thomas M. Orlando¹; Ariel Macatangay³; Prabha Dwivedi¹; Facundo M. Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Thomson Mass Spectrometry Laboratory, UNICAMP, Campinas, Brazil*; ³*NASA Johnson Space Center, Houston, TX*
- TP 730 **Liquid Chromatography Plasma-Spray Ionization-Mass spectrometry (LC-PLASI-MS): Overcoming ESI Limitations;** [Adam Kaylor](#)¹; Prabha Dwivedi¹; Guilong Cheng²; Jian Wang²; Shelly Li²; Jennifer L. Belsky³; Facundo M. Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Pfizer Analytical R&D, Eastern Point Road, CT*; ³*U.S. Pharmacopeial Convention, Rockville, MD*
- TP 731 **Validation of Computational Fluid dynamic Simulations (CFD) with Background Oriented Schlieren technique (BOS);** [Sebastian Klopotoski](#); Alexander Haack; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 732 **Investigation of Gas- and Ion-Dynamics in Heated Glass and Metal Inlet Capillaries: Work in progress ...;** [David Mueller](#); Yessica Brachthaeuser; Valerie Derpmann; Sebastian Klopotoski; Markus Langner; Christine Polaczek; Hendrik Kersten; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 733 **Fundamental Ion-Molecule Reaction Studies at Elevated Ion Temperatures and Analytical Application of an Ion Activation Stage ("ion tunnel");** [Sonja Klee](#); Albrecht Brockhaus; Marco Thinius; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 734 **Development of a Compact Multiple-Ionization-Stage TOF Mass Analyzer System for Trace Component Monitoring within Chemically Challenging Process Gas Matrices;** [Yessica Brachthaeuser](#); David Mueller; Hendrik Kersten; Klaus J. Brockmann; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 735 **Integrated Ion Trajectory Simulations in OpenFOAM, an Open Source Framework for Complex Numerical Simulations;** [Walter Wissdorf](#); Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 736 **An Efficient Ion Funnel Operated at 100 mbar Background Pressure;** [Sascha Albrecht](#)¹; Jochen Barthel¹; Armin Afchine¹; Fred Stroh¹; Thorsten Benter²; ¹*Forschungszentrum Jülich GmbH, Jülich, Germany*; ²*University of Wuppertal, Wuppertal, Germany*
- TP 737 **Kinetic Measurements of Electronically Excited Noble Gas Species Radiating in the Far VUV;** [Ian Barnes](#); Sebastian Klopotoski; Kai Kroll; Hendrik Kersten; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 738 **A Microfabricated Ionizer for High Pressure Mass Spectrometry;** [Craig Cavanaugh](#)¹; Kenion Blakeman¹; Tina Stacy¹; Stanley Pau²; J Michael Ramsey¹; ¹*University of North Carolina, Chapel Hill, NC*; ²*University of Arizona, Tuscon, AZ*
- TP 739 **Coupling Electrospray Ionization with High Pressure Mass Spectrometry;** [William M. Gilliland, Jr.](#); J. Scott Mellors; J. Michael Ramsey; *UNC-Chapel Hill, Chapel Hill, NC*
- TP 740 **Evaluation of Monolithic Silicon-Chip-Based Multinozzle Emitter Arrays for Nano- and Micro-Electrospray Mass Spectrometry;** [Eloy R. Wouters](#)¹; Pan Mao²; Jean-Jacques Dunyach¹; Daojing Wang²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Newomics Inc., Emeryville, CA*
- TP 741 **Preparation and Reactions of Metal Cluster Ions;** [Soumabha Bag](#); Michael Wlekinski; R. Graham Cooks; *Purdue University, West Lafayette, Indiana*
- TP 742 **Characterization and Application of Nanoliter Sample Infusion Into a Miniaturized Liquid Bridge using a Capillary Gap Sampler;** [Volker Neu](#)¹; Pablo Dörig¹; Müller Stephan²; Christof Fattinger²; Renato Zenobi¹; ¹*ETH Zurich, Zurich, Switzerland*; ²*Hoffmann-La Roche AG, Basel, Switzerland*
- TP 743 **Slurry Flow Injection Analysis Coupled with Atmospheric Pressure Chemical Ionization Mass Spectrometry for Quantitative Real-Time Monitoring of Batch Slurry Reactions;** [Zhengqian Zhu](#)¹; David S. Cho²; John E. Bartmess¹; Mary Ellen McNally³; Ron M. Hoffman³; Kelsey D. Cook¹; Ligu Song¹; ¹*Department of Chemistry, University of Tennessee, Knoxville, TN*; ²*Oak Ridge Institute for Science and Education, FBI, Quantico, VA*; ³*Analytical Sciences, DuPont Crop Protection, Newark, DE*
- TP 744 **Detection of Explosives by using a Low Pressure Dielectric Barrier Discharge Ion Source;** [Masuyuki Sugiyama](#); Shun Kumano; Hideki Hasegawa; Kazuki Tanaka; Yuichiro Hashimoto; *Hitachi, Ltd., Tokyo, Japan*
- TP 745 **IR Laser Ablation with Plume Capture by a Continuous Flow Solvent Probe;** [Jeremy T. O'Brien](#)^{1,2}; Evan R. Williams^{1,2}; Hoi-Ying Holman¹; ¹*Lawrence Berkeley National Laboratory, Berkeley, CA*; ²*University of California, Berkeley, Berkeley, CA*
- GCMS: Instrumentation and Applications, 746 - 770**
- TP 746 **Smart Sampling Enables a Fully Automated Workflow for Liquid Injection and Headspace GC and GC/MS;** [Douglas Doster](#)¹; Roger Pearson¹; Tom Flug²; Guenter Boehm²; Brian Peat²; ¹*Aspen Research Corp, Maple Grove, MN*; ²*CTC Analytics, Zwingen, Switzerland*

- TP 747 **A Microfluidic Derivatization Device for GC/MS in Chromatographic Column Chips;** Sanggoo Kim; Sungmin Lim; *Korea Basic Sci. Institute, Seoul, South Korea*
- TP 748 **Laser Ablation Sample Transfer Coupled to Gas Chromatography Mass Spectrometry;** Chinthaka A. Seneviratne; Suman Ghorai; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- TP 749 **Development of a Standard Gas Generating Vial for Performing Quality Control and Evaluation of Portable GC-MS Instrumentation with Solid-Phase Microextraction;** Jonathan Grandy; German Augusto Gómez-Ríos; Janusz Pawliszyn; *University of Waterloo: Pawliszyn Research Group, Waterloo, Canada*
- TP 750 **Improvements in Quantitative and Qualitative Metabolic Profiling using a Novel Atmospheric Pressure GC Source Coupled to High Resolution TOF-MS Analysis;** Christian Wachsmuth¹; Katja Dettmer-Wilde¹; Peter J. Oefner¹; Christoph Gebhardt²; Verena Tellström²; Aiko Barsch²; Thomas Arthen-Engeland²; ¹*University of Regensburg, Regensburg, Germany*; ²*Bruker Daltonik, Bremen, Germany*
- TP 751 **Methods for Improving the Reproducibility of an Atmospheric Pressure Chemical Ionisation Source for Gas Chromatography Analysis;** Gareth Rhys Jones¹; David S Douce²; ¹*Waters UK Ltd, Wilmslow, UK*; ²*Waters (MS Technologies), Manchester, UK*
- TP 752 **Identification of Polycyclic Aromatic Sulfur Heterocycles in Petroleum Using Soft-Ionization GC-QTOFMS;** Viorica Lopez-Avila; Patrick J. Roach; Randall Urdahl; *Agilent Technologies, Santa Clara, CA*
- TP 753 **Exploring the Ionization Space in Traditional EI with high-resolution ToF-MS for Thermally Labile Compounds;** Jonathan Byer; Charles Lyle; Joe Binkley; Jeffrey Patrick; *Leco Corporation, St Joseph, MI*
- TP 754 **Innovative Approach to Helium Carrier Gas Conservation in Analytical Gas Chromatography – Mass Spectrometry;** Alexander Semyonov¹; Massimo Santoro²; Sergio Guazzotti¹; ¹*Thermo Fisher Scientific, Austin, TX*; ²*Thermo Fisher Scientific, Milan, Italy*
- TP 755 **Identification of Co-Eluted Components by High Mass Accuracy and Spectral Accuracy with Quadrupole GC-MS Systems;** Alexander Semyonov¹; Mark Belmont²; Massimo Santoro³; Sergio Guazzotti¹; Ming Gu⁴; Yongdon Wang⁴; ¹*Thermo Fisher Scientific, Austin, TX*; ²*Thermo Fisher Scientific, Schaumburg, IL*; ³*Thermo Fisher Scientific, Milan, Italy*; ⁴*Cerno Bioscience, Norwalk, CT*
- TP 756 **Metabolomic Analysis of Human Plasma by GC-MS;** Yue Luo; Cristina Di Poto; Mohammad R Nezami Ranjbar; Rency Varghese; Chi Zhang; Mahlet Tadesse; Habtom Resson; *Georgetown University, Washington, DC*
- TP 757 **Simultaneous Determination of 20 Kinds of Common Drugs and Pesticides in Human Blood by GPC-GC-MS/MS;** Qian Sun; Changkun Li; Jun Fan; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd, Shanghai, China*
- TP 758 **Quechers Sample Preparation and Gas Chromatography-Tandem Mass Spectrometry Analysis of Multi-Pesticide Residues in Tea and Grain;** Zeying He¹; Shanshan Chen¹; Xiaowei Liu¹; Wenwen Wang²; Chang Liu²; ¹*Agro-Environmental Quality Supervision & Testing, Tianjin, CHINA*; ²*Agilent Technologies Co. Ltd, Beijing, China*
- TP 759 **Headspace GC/MS Analysis of Hydrogen Cyanide in Mainstream Cigarette Smoke;** Megan Mcguigan; LaQuasha Gaddis; Dana Chafin; Sydney Holmberg; Yan Ding; Clifford Watson; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 760 **Identification of Oxygenate Compounds In Gas-to-Olefin Products by Comprehensive Two-Dimensional Gas Chromatography Coupled with Time of Flight Mass Spectrometer;** Junyan Liu; Zhenlei Peng; Jiwen Li; *Sinopec SH. Research Inst. of Petrochemical Tech., Shanghai, China*
- TP 761 **Analysis of Allergens found in Cosmetics using MDGC-GCMS (Multi-dimensional gas chromatography mass spectrometer);** Sanket Chiplunkar; Prashant Hase; Dheeraj Handique; Ankush Bhone; Durvesh Sawant; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India*
- TP 762 **Multi pesticide Residue Analysis in Tobacco by GCMS/MS using QuEChERS as an Extraction Method;** Durvesh Sawant¹; Ankush Bhone¹; Dheeraj Handique¹; Prashant Hase¹; Sanket Chiplunkar¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; Kaushik Banerjee²; Zareen Khan²; ¹*Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*; ²*National Referral Laboratory, NRCG, Pune-412307, Maharashtra, India*
- TP 763 **Analysis of Styrene Leached from Polystyrene Cups using GCMS Coupled with Headspace (HS) Sampler;** Ankush Bhone¹; Dheeraj Handique¹; Prashant Hase¹; Sanket Chiplunkar¹; Durvesh Sawant¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; Nivedita Subhedar²; ¹*Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*; ²*Ramnarain Ruia College, Matunga (E), Mumbai-400019, Maharashtra, India*
- TP 764 **GC-MSMS Characterization of EDCS in Human Tissues for Environmental Risk Factors Assessment in the Sudden Infant and Sudden Intrauterine Death Syndromes;** Pierangela Palma; Veronica Termopoli; Giorgio Famigliani; Fabiana Capriotti; Achille Cappiello; *University of Urbino, Urbino, Italy*
- TP 765 **Simultaneous Determination of Polybrominated Diphenyl Ethers (PBDEs) and Their Hydroxylated Metabolites in Bovine Milk;** Yan-Ping Lin; Katherine Dang; Birgit Puschner; *University of California, Davis, CA*
- TP 767 **Flavor and Aroma Profiles of Truffle Oils by Thermal Desorption GC/MS;** Ronald Shomo; Robert Frey; Christopher Baker; John Manura; *Scientific Instrument Services, Ringoes, NJ*
- TP 768 **Profiling Organic Composition of Art Samples Through HPLC-MS, GC-MS, and Multi-Dimensional Analysis;** Ching Ying Lin¹; Keely Glass¹; Amy Huang¹; Carol Jiang¹; Jen Skerritt¹; George Dubay¹; John Simon²; ¹*Duke University, Durham, NC*; ²*University of Virginia, Charlottesville, VA*
- TP 769 **Analyzing Archaeological Sample Composition through HPLC-MS, GC-MS and Principle Component Analysis;** Amy Huang¹; Keely Glass²; Michael Wei²; Roman Lin²; Carol Jiang²; Jen Skerritt²; Carla Antonaccio²; George Dubay²; ¹*Coral Springs, FL*; ²*Duke University, Durham, NC*
- TP 770 **GCMS as the Ion Chromatograph of the 21st Century: Determination of Inorganic Anions in Matrices of Environmental and Biomedical Interest;** Enea Pagliano¹; Juris Meija¹; Massimo Onor²; Sara Ammazzini²; Emanuela Pitzalis²; Emilia Bramanti²; Alessandro D'Ulivo²; Zoltán Mester¹; ¹*National Research Council Canada, Ottawa, Canada*; ²*Consiglio Nazionale delle Ricerche, Pisa, Italy*
- Polymers, 773 - 792**
- TP 773 **In-line RP-LC-ESI-MS of Gen3 PAMAM Dendrimers;** John R. Lloyd; M. P. Suresh Jayasekara; Kenneth A. Jacobson; *NIH/NIDDK, Bethesda, MD*

- TP 774 **Detecting Peptide and Protein Biomarkers in Serum using Polymeric Reverse Micelles and MALDI-MS Analysis;** [Mahalia Serrano](#); Huan He; Rajasekhar Ramireddy; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- TP 775 **Evaluation of ASAP-IM/MS(MS) Technique for the Characterization of PEEK;** [Emilie Cossoul](#)¹; [Marie Hubert-Roux](#)¹; Muriel Sebban¹; Florence Churlaud²; Hassan Oulyadi¹; Carlos Afonso¹; ¹*University of Rouen - UMR CNRS 6014 Cobra, Mont-Saint-Aignan, FRANCE*; ²*Arkema - CERDATO, Serquigny, France*
- TP 776 **Composition and Architecture of Hyperbranched, Highly Fluorinated Polymers;** [Lydia Cool](#)¹; Matthew Quast²; Anja Mueller²; Chrys Wesdemiotis¹; ¹*The University of Akron, Akron, Ohio*; ²*Central Michigan University, Mount Pleasant, MI*
- TP 777 **Rapid, Simplified Analysis and Data Interpretation of Biodegradable Polymer Mixtures using MALDI-IMMS;** Kirsten Craven; *Waters, Manchester, UK*
- TP 778 **Gas-phase Chemistry of Lithiated Synthetic Polymers: Folding, Charge Solvation and Fragmentation;** Benjamin Bythell; *Univ. of Missouri-St. Louis, St. Louis, MO*
- TP 779 **Negative Ion Electrospray Ionization Mass Spectrometry of Polyglycerol;** [Xiaodong Huang](#); Xiaojin Li; *Ecolab Inc., Naperville, IL*
- TP 780 **Combined Developments in MALDI Mass Spectrometry, Size Exclusion Chromatography and Diffusion NMR for a Successful Characterization of poly(4-vinylpyridine) Molecular Weight;** Christophe Chendo; Marion Rollet; Trang Phan; Stephane Viel; Esra Altuntas; Didier Gigmes; [Laurence Charles](#); *Aix-Marseille University, Marseille Cedex 20, France*
- TP 781 **ESI-MS/MS Structural Characterization of a New Impurity during the Synthesis of PAMAM Dendrimers;** [Aura Tintaru](#); Rémi Ungaro; Xiaoxuan Liu; Laurent Giordano; Ling Peng; Laurence Charles; *Aix-Marseille University, Marseille, France*
- TP 782 **Rapid Analysis of Carbon Fiber Reinforced Plastic using DART-MS;** [Hideaki Kusano](#)¹; Jun Watanabe¹; Yuki Kudou³; Teruhisa Shiota²; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*AMR, Inc., Tokyo, JAPAN*; ³*BioChromato, Fujisawa, Japan*
- TP 783 **Rapid Qualitative and Semi-Quantitative Analysis of PAEs in PVC Samples by Direct Injection Probe APCI High Resolution TOF Mass Spectrometry;** Zhaoyang Liu; *Bruker Daltonics, Inc, Shanghai, China*
- TP 784 **Glycopolymers – Separating Oligomers and Identifying Structural Isomers;** [Sarah Robinson](#); Lydia Cool; Cesar Lopez Gonzalez; Coleen Pugh; Chrys Wesdemiotis; *The University of Akron, Akron, Ohio*
- TP 785 **Characterization of Poly-L-Lysine and Its Noncovalent Complexes by Ion-Mobility- Mass Spectrometry;** [Mehmet Atakay](#)^{1,2}; Bekir Salih²; Chrys Wesdemiotis¹; ¹*Department of Chemistry, The University of Akron, Akron, OH*; ²*Department of Chemistry, Hacettepe University, Ankara, Turkey*
- TP 786 **MALDI-TOF Characterization of α,α -Difunctionalized Poly(ethylene glycol) for Bioconjugate Synthesis;** C. Adrian Figg; [Maria Cristina A. Dancel](#); Bryan S. Tucker; Brent S. Sumerlin; *University of Florida, Gainesville, FL*
- TP 787 **Quantitative Analysis of Bulk and Extractable PVP incorporated in Silicone Hydrogel Contact Lenses using APCI HR/AM-SIM Mass Spectrometry;** [William Nichols](#)¹; Andrew J. Hoteling²; Lawrence Salvati III^{2,2}; Patricia Harmon²; ¹*Mass2Charge Consulting LLC, Newark, NY*; ²*Bausch+Lomb, Rochester, NY*
- TP 788 **Structural and Mixture Characterization of Polysorbate 60 using GPC-Spray Deposition and MALDI-ToF MS;** Mark Arnould; *Xerox, Webster, NY*
- TP 789 **Direct Analysis in Real Time (DART) Ion Trap Mass Spectrometry for Detection and Identification of poly(dimethylsiloxane) Polymers on Surfaces;** [Curtis Mowry](#); Michael Brumbach; Adam Pimentel; Alex Mirabal; *Sandia National Laboratories, Albuquerque, NM*
- TP 790 **Characterization of Homo-arm and Mikto-arm Poly(ethylene Glycol) Stars using Vacuum Ionization-Ion Mobility Spectrometry-Mass Spectrometry;** [Casey Foley](#)¹; Tarick El-Baba¹; Boyu Zhang²; Scott Grayson²; Sarah Trimpin¹; ¹*Wayne State University, Detroit, MI*; ²*Tulane University, New Orleans, LA*
- TP 791 **Comprehensive Analysis of Extractable from Rubber Stopper used in Medical Devices and Pharmaceutical Products;** [Andrew Feilden](#)¹; Amalendu Sarkar²; Kate Comstock³; ¹*Smithers Rapra, Shrewsbury, UK*; ²*Qure Medical, Rock Hill, SC*; ³*Thermo Fisher Scientific, San Jose, CA*
- TP 792 **Comparing Additives and other Extractables from Primary and After-Market Cell Phone Cases by Gas Chromatography-Time of Flight Mass Spectrometry;** [Christina Nieh](#)¹; Joe Binkley²; ¹*LECO Corporation, Saint Joseph, MI*; ²*LECO Corporation, St. Joseph, MI*



7:30 – 8:00 am..... Set up all Wednesday posters
 10:30 am – 1:00 pm..... Odd-numbered posters present
 12:00 – 2:30 pm..... Even-numbered posters present
 7:30 – 8:00 pm..... Remove all Wednesday posters

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- WP 001 **Highly Robust Sample Preparation with 2,5-dihydroxyacetophenone for MALDI Imaging of Proteins (2 -70 kDa) at High Spatial Resolution (5 µm);** Junhai Yang; Andre Zavalin; Richard Caprioli; Vanderbilt University, Nashville, TN
- WP 002 **Digging Deeper: Using Acid-Cleavable Detergents to Uncover More of the MSI Proteome;** Peggi Angel; Erin H. Seeley; Gregory Boyce; Greg W. Kilby; Protea Biosciences, Inc., Morgantown, WV
- WP 003 **Photo-Thermal Decomposition/Digestion (Photo-TDD) of Proteins and Its Application in MALDI-MS Imaging;** Rong Zhou; Franco Basile; University of Wyoming, Laramie, WY
- WP 004 **Infrared Laser Ablation Sample Transfer with On-Target Digestion for MALDI Imaging;** Fan Cao; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- WP 005 **Imaging MALDI MS of Dosed Mouse Brain Utilizing Novel Sample Preparation Technique;** Cristine Quiason; Sheerin K. Shahidi-Latham; Justin Q. Ly; Edna F. Choo; Genentech Inc., South San Francisco, CA
- WP 006 **In-Depth Characterization of the Neuropeptidome in Crustacean Stomatogastric Nervous System by Imaging Mass Spectrometry on an Orbitrap Platform;** Chuanzi Ouyang¹; Bingming Chen²; Albert Kim³; Lingjun Li^{1,2}; ¹Department of Chemistry, UW-Madison, Madison, WI; ²School of Pharmacy, UW-Madison, Madison, WI; ³Department of Biochemistry, UW-Madison, Madison, WI
- WP 007 **A High Throughput Method for Mass Spectrometric Profiling of Glycomics and Proteomics from Tissue Microarrays;** Chun Shao; Lilla Turiák; Le Meng; Qi Wang; Nancy Leymarie; Cheng Lin; Joseph Zaia; School of Medicine, Boston University, Boston, MA
- WP 008 **Simultaneous Proteomics and Glycomics Profiling from Histological Tissue;** Lilla Turiák; Le Meng; Chun Shao; Kshitij Khatri; Nancy Leymarie; Qi Wang; Joseph Zaia; Boston University School of Medicine, Boston, MA
- WP 009 **High-resolution Ambient Mass Spectrometry Imaging of Mouse Tissues by Surface Micro-Extraction using the Single-probe;** Wei Rao; Ning Pan; Renmeng Liu; Zhibo Yang; University of Oklahoma, Norman, OK

- WP 010 **Heat Fixation Inactivates Viral and Bacterial Pathogens and is Compatible with Downstream MALDI Mass Spectrometry Tissue Imaging;** Lisa H. Cazares^{1,2}; Sean Vantongeren³; Tara Kenny³; Douglas Lane³; Rekha Panchal³; Sina Bavari³; ¹Henry M. Jackson Foundation, Frederick, MD; ²DoD, BHSI, Fredrick, MD; ³USAMRIID/ Molecular and Translational Sciences, Frederick, MD
- WP 011 **Investigating the Use of Heat Stabilization during Sample Preparation of Tissues for Mass Spectrometry Imaging;** Suzanne Robertson¹; Jeremy Barry¹; Guillaume Robichaud¹; Nagendran Muthusamy¹; Craig Sykes²; Corbin Thompson²; Troy Ghashghaei¹; Angela Kashuba²; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 012 **High Quality Sections and Molecular Distribution Images of Neuropeptides From Heat Stabilized Tissue;** Mats Borén¹; Olof Sköld¹; Anna Nilsson²; Richard Goodwin^{2,3}; Per E. Andren²; ¹Denator AB, Uppsala, Sweden; ²Uppsala University, Uppsala, Sweden; ³AstraZeneca, Macclesfield, UK
- WP 013 **Measuring MALDI: Investigating MALDI Fundamentals with ToF-SIMS;** Melissa K. Passarelli¹; Ian S. Gilmore¹; Josephine Bunch¹; Peter Marshall²; Sophie Myhill²; Andy West²; ¹National Physical Laboratory, Teddington, U.K.; ²GlaxoSmithKline, Stevenage, U.K.

Informatics: Profile Analysis, 014 - 023

- WP 014 **Comprehensive Characterization of the Secretome of CNS Cell Lines using High-Resolution LC-MS/MS;** Jongmin Woo¹; Dohyun Han²; Youngsoo Kim²; ¹Department of Biomedical Sciences, SNU, Seoul, Korea; ²Department of Biomedical Engineering, SNU, Seoul, Korea
- WP 015 **An Extensive and Reproducible Ion-Current-based Proteomic Profiling Provided New Insights into the Understanding the Mechanism of Myogenic Differentiation;** Jun Qu¹; Chengjian Tu¹; Jun Li¹; Shichen Shen¹; James Clements²; yahao Bu²; David Hangauer²; ¹University at Buffalo, Buffalo, NY; ²Kinex Pharmaceuticals LLC, Buffalo, NY
- WP 016 **The Omics Evidences: Single Nucleotide Variants Transmissions on Chromosome 20 in Liver Cancer Cell Lines;** Quanhui Wang^{1,2}; Bo Wen²; Shaohang Xu²;

- Zhe Ren²; Guixue Hou^{1,2}; Ruo Zhou^{2,2}; Jin Zi²; Xiaomin Lou¹; Haidan Sun¹; Fan Zhong³; Qingyu He⁴; Ping Xu⁵; Liang Lin²; Siqi Liu^{1,2}; ¹Beijing Institute of Genomics, CAS, Beijing, China; ²BGI-Shenzhen, Shenzhen, China; ³Fudan University, Shanghai, China; ⁴Jinan University, Guangzhou, China; ⁵Beijing Proteome Research Center, Beijing, China
- WP 017 **A Cloud Computing Implementation of Differential Mass Spectrometry: A Label Free Method for Proteomic Profiling;** Nathan Yates¹; Christine Wu²; Michael J. Maccoss³; Andrey Bondarenko⁴; ¹University of Pittsburgh, Pittsburgh, PA; ²University of Pittsburgh School of Medicine, Pittsburgh, PA; ³Univ of Washington, Seattle, WA; ⁴InfoClinika, Bellevue, WA
- WP 018 **mTMT-visHTS: A Novel Method for Multiplexing TMT Datasets with a Tunable Visualization High Throughput Screening Software for Easy Protein Profiling;** Piero Ricchiuto¹; Katsumi Yabusaki^{1,2}; Hiroshi Iwata¹; Iwao Yamada^{1,2}; Masanori Aikawa¹; Sasha Singh¹; ¹Harvard Medical School & BWH, Boston, MA; ²Kowa Company, Ltd., Tokyo, Japan
- WP 019 **The Modelling and Poisson Harvesting of LC-MS Spectra;** Edmond Breen; *APAF, Sydney, AUSTRALIA*
- WP 020 **Automated Classification and Visualization of Histological Features by Mass Spectrometry Imaging;** Ottmar Golf^{1,2}; Nazanin Zounemat Kermani¹; Sabine Guenther^{1,2}; Robert D. Goldin¹; James Kinross¹; Abigail V. M. Speller¹; Zoltan Takats¹; Kirill Veselkov¹; ¹Imperial College London, London, UK; ²Justus Liebig University, Giessen, Germany
- WP 021 **An Informatics Approach for Evaluating and Guiding Method Development for Biomarker;** Y. Melodie Du¹; R. Graham Cooks¹; Yu Xia¹; Ye Hu²; Zheng Ouyang¹; ¹Purdue University, West Lafayette, IN; ²The Methodist Hospital Research Institute, Houston, TX
- WP 022 **The Use of Fragment Ion and Collision Cross Section for Confident Identification from LC-Ion Mobility-MS Metabolomics Data;** Giorgis Isaac¹; Giuseppe Astarita¹; Steven Lai¹; Adam Ladak¹; James Langridge³; John Shockcor¹; Andy Borthwick²; ¹Waters Corporation, Milford, MA; ²Nonlinear Dynamics, Newcastle, UK; ³Waters Corporation, Manchester, UK
- WP 023 **Automated Glycan Assignment using Accurate Mass Measurement with a Calibrated Retention Time in Glucose Units;** Ying-Qing Yu¹; Weibin chen¹; Mark Hilliard²; Niaobh McLoughlin²; Pauline Rudd²; ¹Waters Corporation, Milford, MA; ²NIBRT, Dublin, Ireland
- Informatics: General, 024 - 037**
- WP 024 **Application of Performance Metrics Software for Optimization of Proteomics Data Acquisition;** David Mccaskill; Yaw Nti-Addae; Suresh Babu Annangudi Palani; Tao Xu; Jeffrey Gilbert; *Dow AgroSciences, Indianapolis, IN*
- WP 025 **An Innovative Software Platform for the Visualization of Routine GC and LC-MS Data;** David Hardy¹; Vitaly Lashin²; Pranas Japertas³; ¹ACD/Labs, Bracknell, UK; ²ACD/Labs, Moscow, Russia; ³ACD/Labs, Vilnius, Lithuania
- WP 026 **Reconstruction of Mass Spectra Using Fuzzy Optimal Associative Memories (FOAMs);** Zhengfang Wang; Mengliang Zhang; Peter Harrington; *Ohio University, Athens, Ohio*
- WP 027 **Carbocationic Mass Tags for Information Encoding and Multiplex Bioanalytical Applications;** Artyom Topolyan¹; Vladimir Brylev¹; Alexey Ustinov²; Andrey Formanovsky¹; Vladimir Korshun¹; ¹Institute of Bioorganic Chemistry RAS, Moscow, Russia; ²Lumiprobe Corporation, Hallandale Beach, FL
- WP 028 **Analysis of Longitudinal Serum Proteomics Profiles from Studies of a T1D-risk Cohort;** Robert Moulder¹; Santosh Bhosale¹; Heikki Hyöty^{2,3}; Riitta Veijola⁴; Mikael Knip^{5,6}; Jorma Ilonen^{7,8}; Tuula Simell¹⁰; Jorma Toppari^{1,12}; Harri Lähdesmäki¹¹; Olli Simell¹⁰; Riitta Laheesmaa¹; David Goodlett^{1,9}; ¹Turku Centre for Biotechnology, Turku, Finland; ²School of Medicine, University of Tampere, Tampere, Finland; ³Fimlab Laboratories, Pirkanmaa Hospital District, Tampere, Finland; ⁴Dept. of Pediatrics, Uni. of Oulu & Central Hospital, Oulu, Finland; ⁵Dept. Pediatrics, Helsinki Uni. Central Hospital, Helsinki, Finland; ⁶Dept. of Pediatrics, Tampere University Hospital, Tampere, Finland; ⁷Dept. of Clinical Microbiology, Uni. Eastern Finland, Kuopio, Finland; ⁸Immunogenetics Laboratory, University of Turku, Turku, Finland; ⁹University of Maryland, Baltimore, MD; ¹⁰Department of Pediatrics, University of Turku, Turku, Finland; ¹¹Aalto University School of Science, Espoo, Finland; ¹²Department of Physiology, University of Turku, Turku, Finland
- WP 029 **PEFF: A Common Sequence Database Format in Proteomics;** Pierre-Alain Binz¹; Eugene Kapp²; Jim Shofstahl³; David Creasy⁴; Lydie Lane⁵; Robert Chalkley⁶; Matt Chambers⁷; Harald Barsnes⁸; Sean L. Seymour⁹; ¹CHUV, Lausanne, Switzerland; ²Ludwig Institute for Cancer Research, Melbourne, Australia; ³Thermo Fisher Scientific, San Jose, CA; ⁴Matrix Science Ltd, London, United-Kingdom; ⁵Swiss Institute of Bioinformatics, Geneva 4, Switzerland; ⁶UCSF, San Francisco, CA; ⁷Vanderbilt University, Nashville, TN; ⁸University of Bergen, Bergen, Norway; ⁹AB Sciex, Foster City, CA
- WP 030 **Automated Mass Shift Detection, Accurate Peak Area Integration, Identification and Relative Quantification of INLIGHT™ Derivatized N-Glycans for LC-MS Comparative Glycomics;** Kenneth Garrard; Amber Cook; Guillaume Robichaud; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- WP 031 **Critical Assessment of the Elemental Isotope Definition in Mass-Spectrometry-Based Proteomics;** Jürgen Claesen¹; Frank Sobott³; Tomasz Burzykowski¹; Dirk Valkenborg²; ¹Hasselt University, Diepenbeek, Belgium; ²VITO, Mol, Belgium; ³CFP-CeProMa, University of Antwerp, Antwerp, Belgium
- WP 032 **Identification of Non-Synonymous SNP Products to Search High Resolution Tandem Mass Spectra Against a Novel Protein Database;** Carol Nilsson¹; Cheryl Lichti¹; Ekaterina Mostovenko¹; Fabrizio Donnarumma²; Melinda Rezel³; György Marko-Varga³; Akos Vegvari³; ¹UTMB, Galveston, TX; ²Louisiana State University, Baton Rouge, LA; ³Lund University, Lund, Sweden
- WP 033 **The Probabilistic Convolution Tree: A Dynamic Programming Algorithm for Sub-Quadratic Inference with Generic Causal Graphical Models;** Oliver Serang; *Thermo Fisher Scientific, Bremen, Germany*
- WP 034 **GradientOptimizer: An Open-Source Graphical Environment for Calculating Optimized Gradients in Reversed-Phase Liquid Chromatography;** Luminita Moruz¹; Lukas Käll²; ¹Stockholm University, Stockholm, Sweden; ²Royal Institute of Technology, Stockholm, Sweden
- WP 035 **McFine - An Algorithm to Approximate the Isotope Fine Structure of Peptides and Proteins;** Piotr Dittwald¹; Dirk Valkenborg^{2,3}; Alan L. Rockwood^{4,5}; Anna Gambin¹; ¹University of Warsaw, Warsaw, Poland; ²VITO, Mol, Belgium; ³I-Biostat, Hasselt University, Diepenbeek, Belgium; ⁴ARUP Laboratories, Salt Lake City, UT; ⁵Department of Pathology, University of Utah, School of Medicine, Salt Lake City, UT

- WP 036 **Persistent Myths and Uncomfortable Truths: Taking MS-omics Data Processing from the Emperor's New Clothes to a Rigorous Science**; Rob Smith¹; Dan Ventura; John Prince; *Brigham Young University, Provo, UT*
- WP 037 **CHORUS: A Community Based Solution for the Storage, Analysis, and Exchange of Mass Spectrometry Data and Information**; Andrey Bondarenko¹; Michael J. Maccoss²; Christine Wu⁴; Nathan Yates³; ¹*InfoClinika, Bellevue, WA*; ²*Univ of Washington, Seattle, WA*; ³*University of Pittsburgh, Pittsburgh, PA*; ⁴*University of Pittsburgh School of Medicine, Pittsburgh, PA*
- Informatics: Peptide Identification and Characterization, 038 - 054**
- WP 038 **Altered Fragmentation Patterns in Amidinated Tryptic Peptides Enhance Peptide Identification**; Sujun Li; Suraj Saraswat; James P. Reilly; Haixu Tang; Predrag Radivojac; *Indiana University, Bloomington, IN*
- WP 039 **Cleaved and Missed Sites for Trypsin, Lys-C, Lys-N can be Predicted with High Confidence on the Basis of Sequence Context**; Andrew J Alpert²; Paul Gershon¹; ¹*UC-Irvine, Irvine, CA*; ²*PolyLC Inc., Columbia, MD*
- WP 040 **Improving the Accuracy of Peptide Retention Time Prediction by Machine Learning Techniques**; Bob Xiong; Susan Deupree; Brian Nofsinger; Mike Allen; *Tandem Labs - RTP, Durham, NC*
- WP 041 **Rapid Characterization, Annotation and Comparison of Peptide Maps**; Michael Kim¹; Yong Kil²; Marshall Bern²; Chris Becker²; Richard Seipert¹; ¹*Genentech, South San Francisco, CA*; ²*Protein Metrics, San Carlos, CA*
- WP 042 **Pattern Detection in Associated Artifact Peaks in Mass Spectra with Frequent Itemset Mining**; Trung Nghia Vu^{1,4}; Dirk Valkenborg^{2,3}; Evelyne Maes^{2,3}; Filip Lemièrè^{1,3}; Bart Goethals¹; Kris Laukens^{1,4}; ¹*University of Antwerp, Antwerp, Belgium*; ²*VITO, Mol, Belgium*; ³*Centre for Proteomics, University of Antwerp, Antwerp, Belgium*; ⁴*biomina, Antwerpen, Belgium*
- WP 043 **Rule Based Peak Filtering of High Mass Accuracy MS/MS-spectra Improves Peptide Identification Rates**; Jakob Bunkenborg¹; Per Hägglund²; Henrik Molina³; ¹*Copenhagen University Hospital, Hvidovre, Denmark*; ²*Technical University of Denmark, Kgs. Lyngby, Denmark*; ³*The Rockefeller University, New York, NY*
- WP 044 **Removing Isobaric-Related Ions Significantly Improves the Peptide/Protein Identification Sensitivity of High Resolution MS/MS Data**; Quanhu Sheng¹; Rongxia Li²; Jie Dai³; Qingrun Li²; Chen Li²; Zhiduan Su²; Yu Shyr¹; Rong Zeng²; ¹*Vanderbilt University, Nashville, TN*; ²*Shanghai Institutes for Biological Sciences, Shanghai, China*; ³*University of Southern Denmark, Odense, Denmark*
- WP 045 **Improving Protein and Peptide Identification in Tandem Mass Spectrometry by Peptide Search Space Reduction**; Avinash Shanmugam; Chih-Chiang Tsou; Dmitry Avtonomov; Anastasia Yocum; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- WP 046 **A Fast Filtering Method for Peptide Identification by Blocked Pattern Matching**; Fei Deng¹; Xiaowen Liu²; Lusheng Wang¹; ¹*Dept. of Computer Science, City Univ. of Hong Kong, Hong Kong, China*; ²*IUPUI, Indianapolis, IN*
- WP 047 **A Chromatography Independent 2-Phase Algorithm for Increasing DDA Protein Identifications by up to 80% and Peptide Identifications by 200%**; David Scigocki¹; Christian Claude¹; Patrick Vayn¹; Elie Abenmoha^{1,2}; John Lindsay^{1,3}; David Znaty¹; John Asara^{4,5}; ¹*Physikron, Inc., Paris, FR*; ²*Me Conseil, Paris, FR*; ³*SciPartners, Inc., Westford, MA*; ⁴*Beth Israel Deaconess Medical Center, Boston, MA*; ⁵*Harvard Medical School, Boston, MA*
- WP 048 **fishTones.js: Interactive Peptide MSMS Characterization in Non-Traditional Proteomic Workflows**; Alexandre Masselot; Victoria Pham; Lilian Phu; Tobias Maile; Wendy Sandoval; Donald Kirkpatrick; David Arnott; *Genentech, South San Francisco, CA*
- WP 049 **PeptideAnalyzer: An Integrated Platform for Efficient In-Depth Characterization of Therapeutic Proteins**; Vincent Larrailet¹; Georg Drabner¹; Amy Hilderbrand²; Maximiliane Hilger¹; Tobias Kailich³; Michael Kim²; Hans Koll¹; Wilma Lau¹; Ingo Lindner³; Michael Molhoj¹; Richard Seipert²; X. Christopher Yu²; Hans Rainer Voelger¹; ¹*Pharma Research, Roche Diagnostics GmbH, Penzberg, Germany*; ²*Protein Analytical Chemistry, Genentech, South San Francisco, United States*; ³*Pharma Biotech Development, Roche Diagnostics GmbH, Penzberg, Germany*
- WP 050 **Software Tools to Accelerate Peptide Mapping and Related Analysis for Characterizing Biotherapeutics**; Joe Shambaugh¹; Peter Haberl²; Alessio Ceroni²; Arnd Brandenburg³; Jens Hoefkens¹; ¹*Genedata Inc., Lexington, MA*; ²*Genedata GmbH, Martinsried, Germany*; ³*Genedata AG, Basel, Switzerland*
- WP 051 **Creation of a Tandem MS HCD Spectral Library for Identification of Peptides and Modifications of a Therapeutic Monoclonal Antibody**; Qian Dong; Xinjian Yan; Yuri Mirokhin; Yuexue Liang; Stephen Stein; *NIST, Gaithersburg, MD*
- WP 052 **Scrambling and Enumeration Modules Developed for the Structure Elucidation of MSⁿ Data Utilizing the MASSPEC Algorithm**; Marshall M. Siegel; Gary Walker; *MS Mass Spec Consultants, Fair Lawn, NJ*
- WP 053 **pParse 2.0: A Faster and More Sensitive Algorithm for Detection of Monoisotopic Peaks**; Long Wu¹; Wen-Feng Zeng¹; Zuo-Fei Yuan¹; Kun Zhang¹; Jia-Ming Meng¹; Sheng-Bo Fan¹; Chao Liu¹; Hao Chi¹; Lai-Yun Qing²; Rui-Xiang Sun¹; Si-Min He¹; ¹*Institute of Computing Technology, CAS, Beijing, China*; ²*School of Computer and Control Engineering, UCAS, Beijing, China*
- WP 054 **pFind: Fast and Comprehensive Analysis of High Resolution MS Data**; Hao Chi; Wen-Feng Zeng; Long Wu; Kun He; Chao Liu; Rui-Xiang Sun; Si-Min He; *Institute of Computing Technology, CAS, Beijing, China*
- Intact Proteins: PTM Discovery, 055 - 059**
- WP 055 **LC-MS Analysis of Intact Enzymes using the Synapt G2 Mass Spectrometer**; Ioana Barbu; Nicolas Abello; Jort Gerritsma; Marcel van Tilborg; Maurien Olsthoorn; *DSM Biotechnology Center, Analysis department, Delft, Netherlands*
- WP 056 **Structural Determination of Different Protein Phosphoforms**; Matthias Vonderach¹; Francesco Lanucara¹; Ben Cossins²; Claire Eyers¹; ¹*Institute of Integrative Biology, Liverpool, UK*; ²*UCB, Slough, UK*
- WP 057 **Comprehensive Characterization of Molecular Heterogeneities in α -actins from Cardiac Tissues by Top-Down Mass Spectrometry**; Serife Ayaz Guner²; Ying Peng²; Ivy Chen²; Ying Ge^{1,2}; ¹*Cell and Regenerative Biology, Madison, WI*; ²*University of Wisconsin - Madison, Madison, WI*
- WP 058 **Targeted Protein Enrichment by Intact Protein SRM and Fraction Collection to Enable PTM-Based Biomarker Discovery from CSF of Individual Patients**; Junmei Zhang; Daniel Plymire; John Corbett; Steven Patrie; *UT Southwestern, Dallas, TX*
- WP 059 **Complete Post-Translational Modification Mapping of Pilins from Clinical Strains of Pathogenic *Neisseria meningitidis* Requires Top-Down Mass Spectrometry**; Joseph Gault¹; Christian Malosse^{1,2}; Marie-Cécile Ploy⁶;

Catherine E. Costello³; Guillaume Dumenil^{4,5}; Julia Chamot-Rooke^{1,2}; ¹Institut Pasteur, Paris, France; ²CNRS UMR3528, Paris, France; ³Boston University School of Medicine, Boston, MA; ⁴INSERM U970, Paris, France; ⁵Université Paris Descartes, Paris, France; ⁶INSERM UMR1092, Limoges University Hospital, Limoges, France

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- WP 060 **Analysis of Serum Haptoglobin Fucosylation in Hepatocellular Carcinoma and Liver Cirrhosis of Different Etiologies;** Jianhui Zhu¹; Zhenxin Lin¹; Jing Wu¹; Haidi Yin¹; Jianliang Dai²; Ziding Feng²; Jorge Marrero³; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Texas MD Anderson Cancer Center, Houston, TX; ³UT Southwestern Medical Center, Dallas, TX
- WP 061 **Ultracentrifugation-based Glycoproteomic: Approach for Discovery of Plasma Glycoprotein Markers;** Esther Cheow; NTU, Singapore, Singapore
- WP 062 **A Comparative Glycoproteome Study of Developing Endosperm in the Hexose-Deficient *miniature1* Seed Mutant and Its Wild Type Mn1 in maize;** Cecilia Silva-Sanchez¹; Jinxi Li¹; Sixue Chen^{1,2}; Prem Chourey³; ⁴ICBR-Proteomics UF, Gainesville, FL; ²University of Florida, Gainesville, FL; ³USDA-Agricultural Research Service, CMAVE, Gainesville, FL; ⁴Department of Agronomy, UF, Gainesville, FL
- WP 063 **Improved Glycopeptide Analysis using Acetonitrile Enriched Sheath Gas and Oxonium Ion Dependent ETD;** Kristina Marx; Andrea Kiehne; Markus Meyer; Bruker Daltonik GmbH, Bremen, Germany
- WP 064 **Identification of Complex Glycopeptides using Tandem Mass Spectra;** Yanlin Zhang¹; Chuan-Yih Yu²; Shuaicheng Li³; Haixu Tang²; Xiaowen Liu¹; ¹IUPUI, Indianapolis, IN; ²Indiana University, Bloomington, IN; ³City University of Hong Kong, Hong Kong, China
- WP 065 **Comprehensive Analysis of Recombinant Human Erythropoietin Glycoforms by Capillary Electrophoresis and Nanoflow Liquid Chromatography Coupled with Middle-Down Mass Spectrometry;** Rosa Viner¹; Anthonius A.M. Heemskerk²; David M Horn¹; Julian Saba¹; Marshall W. Bern³; David R Bush⁴; Marcia R Santos⁵; Hans Dewald⁶; Alexander R. Ivanov⁴; Barry L. Karger⁴; ¹ThermoFisher Scientific, San Jose, CA; ²Leiden University Medical Center, Leiden, Netherlands; ³Protein Metrics, Palo Alto, CA; ⁴Barnett Inst., Northeastern University, Boston, MA; ⁵AB Sciex LLC, Brea, CA
- WP 066 **Online Enrichment and Decoupled LC Separation of Sialylated/Phosphorylated Glycans and Glycopeptides;** Serenus Hua¹; Gregory Staples²; Youngsuk Seo¹; Myung Jin Oh¹; Rudolf Grimm²; Hyun Joo An¹; ¹AGRS, Chungnam National University, Daejeon, Korea; ²Agilent Technologies, Santa Clara, CA
- WP 067 **Dynamics of Residue-Specific Chromatin O-GlcNAcylation *in vivo*;** Xiaoshi Wang; Benjamin A Garcia; University of Pennsylvania, Philadelphia, PA
- WP 068 **A Seamless Workflow for Comprehensive Analysis of the Mucin-Type O-linked Glycoproteome;** Jun Zhu¹; Kai Cheng¹; Jin Wenhai²; Fangjun Wang¹; Mingming Dong¹; Mingliang Ye¹; Christie Hunter³; Hanfa Zou¹; ¹Dalian Institute of Physical Chemistry, Dalian, China; ²AB SCIEX China, Shanghai, China; ³AB SCIEX, USA, Foster City, CA
- WP 069 **The Identification and Characterization of a General Protein O-glycosylation System within the Burkholderia cepacia Complex;** Nichollas Scott¹; Julian Saba²; Helene Cardasis³; Leonard Foster¹; Jon Dennis⁴; ¹University of British Columbia, Vancouver, Canada; ²Thermo Fisher Scientific, Montreal, QC; ³Thermo Scientific, New York, NY; ⁴University of Alberta, Edmonton, Canada
- WP 070 **A Data-Independent Acquisition Strategy on the Q Exactive for Monitoring GALNT2- mediated APOCIII Glycosylation in Cell Culture;** Iwao Yamada^{1,2}; Hideo Yoshida^{1,2}; Sasha A. Singh¹; Masanori Aikawa¹; ¹Brigham and Women's Hospital, Boston, MA; ²Kowa Company, Ltd., Tokyo, Japan
- WP 071 **Characterization of O-GlcNAc Modified Sites on the RUNX2 Osteogenic Transcription Factor;** Alexis Nagel; Lauren Ball; MUSC, Charleston, SC
- WP 072 **A Multiple Reaction Monitoring Method to Specifically Characterize and Relatively Quantify the O-glycans of the Potential Biologic Lubricin;** Sarah Flowers¹; Catherine Lane²; Liaqat Ali¹; Tannin Schmidt³; Niclas Karlsson¹; ¹Gothenburg University, Gothenburg, Sweden; ²AB Sciex, Warrington, UK; ³University of Calgary, Calgary, Canada
- WP 073 **Characterization of O-glycosyltransferase Reactions at the Molecular Level using nanoLCMS;** Tyler Stewart¹; Kazuo Takahashi²; Milan Raska³; Milada Stuchlova Horynova³; Jan Novak¹; Matthew B. Renfrow¹; ¹University of Alabama at Birmingham, Birmingham, AL; ²Fujita Health Univ., Toyoake, Japan; ³Palacky University, Olomouc, Czech Republic
- WP 074 **Identification and Profiling of O-Glycans in Human Factor Xa by Advanced LC-MS/MS Techniques;** Jeremy Woods; Song Klapoetke; Michael Xie; KBI Biopharma, Durham, NC - North Carolina
- WP 075 **Glycopeptide CID MS/MS Analysis for Elucidation of the Impact of a Single Nucleotide Polymorphism on O-Glycan Microheterogeneity in Glycoprotein ITIH4;** Kevin B Chandler¹; Miloslav Sanda²; Zuzana Brnakova²; Nathan Edwards³; Radoslav Goldman²; ¹Boston University, Boston, MA; ²Georgetown University, Lombardi Cancer Center, Washington, DC; ³Georgetown University, Department of Biochemistry, Washington, DC
- WP 076 **Applying improved ionization Procedures for O-glycopeptide Characterization of Arabinogalactan Protein 31 (AGP31) by Combined CID and ETD Fragmentation;** Kristina Marx¹; Cecile Albenne²; Guillaume Tremintin³; Ulrike Schweiger-Hufnagel¹; Pierre-Olivier Schmit⁴; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Université de Toulouse, Castanet-Tolosan, France; ³Bruker Daltonics, Fremont, CA; ⁴Bruker Daltonique S.A, Wissembourg, France
- WP 077 **Comprehensive N-glycomic Analysis of Clear Cell Renal Cell Carcinoma Plasma using Lectin Affinity HPLC Fractionation and Porous Graphitized Carbon LC-ESI-MS/MS;** Francisca Gbormittah¹; William Hancock¹; Othon Iliopoulos²; ¹Northeastern University, Boston, MA; ²Harvard Medical School, Boston, MA
- WP 078 **Sequential Ion Mobility Resolved Electron Transfer Dissociation and Collision Induced Dissociation of N-Glycopeptides;** Venkata Kollu¹; Eric D. Dodds²; ¹Univ of Nebraska Lincoln, Lincoln, NE; ²University of Nebraska - Lincoln, Lincoln, NE
- WP 079 **N-glycome Characterization of Secreted N-glycoproteins from a Panel of Eight Breast Cell Lines using Porous Graphitized (PGC) Carbon LC-MS/MS Analysis;** Ling Y. Lee¹; Morten Thaysen-Andersen¹; Mark S. Baker¹; Nicole H. Packer¹; William S. Hancock^{1,2}; Fanayan Susan¹; ¹Macquarie University, Sydney, Australia; ²Northeastern University, Boston, MA

- WP 080 **Targeting the N-Linked Glycome**; Ron Orlando¹; Shujuan Tao¹; Yining Huang¹; Alex Harvey²; Barry Boyes³; ¹University of Georgia, Athens, GA; ²GlycoScientific, LLC, Athens, Georgia; ³Advanced Materials Technology Inc., Wilmington, DE
- WP 081 **The Effect of Antibody N-Glycosylation on FcRn Binding**; Jake Pawlowski¹; Tyler Carlage²; Adriana Bajardi-Taccioli²; Damian Houde²; Marina Feschenko²; Li Zang²; Yelena Lyubarskaya²; ¹UMASS Amherst, Amherst, Massachusetts; ²Biogen Idec, Cambridge, MA
- WP 082 **N-glycosylation Analysis in Human Scavenger Receptor CD36 by HCD Product Ion-Triggered ETD Mass Spectrometry**; Cleidiane G. Zampronio¹; David J. Sanders²; Kenneth J. Linton²; Andrew J. Creese¹; Helen J. Cooper¹; ¹School of Biosciences, University of Birmingham, Birmingham, UK; ²Blizard Institute, Queen Mary University, London, UK
- WP 083 **High Speed HILIC HPLC for Glycan Analysis**; James Martosella¹; Chris Rogers²; Oscar Potter³; Jia Liu¹; ¹Agilent Technologies, Wilmington, de; ²Agilent Technologies, Shropshire, UK; ³Agilent Technologies, Santa Clara, CA
- WP 084 **Displacement Phenomena in Serial Lectin Affinity Chromatography**; Wonryeon Cho; Wonkwang University, Iksan, Republic of Korea
- WP 085 **Comparative Glycoproteomics Analysis of Influenza Virus Hemagglutinin using a Multidimensional LC-MS/MS Based Workflow**; Kshiti Khatri; Nancy Leymarie; Joseph Zaia; Boston University, Boston, MA
- WP 086 **Comprehensive Site-Specific Characterization of Glycoproteins using Enzymes of Varying Cleavage Specificities**; Carlito Lebrilla; Evan Parker; Michael Xin Sun; Jincui Huang; Andres Guerrero; UC Davis, Davis, CA
- WP 087 **Absolute Quantitation of Human Milk Proteins and Their Glycoforms using Multiple Reaction Monitoring (MRM)**; Jincui Huang; Qiuting Hong; Rocchina Sabia; Carlito Lebrilla; UC Davis, Davis, CA
- WP 088 **An Integrated Top-Down and Bottom-Up Approach for Intact Glycoprotein Analysis of Aspergillus niger Secretome**; Yi Qu¹; Li Cao²; Ju Feng¹; Zhaorui Zhang¹; Erika Zink¹; Rui Zhao¹; Shuang Deng¹; Yuxuan Jiang¹; Nikola Tolic¹; Da Meng¹; Uma Aryal³; Ljiljana Paša-Tolić¹; Weijun Qian¹; Marshall W. Bern⁴; Qibin Zhang¹; Mary Lipton¹; Jian-Zhi Hu¹; Scott Baker¹; Si Wu¹; ¹PNPL, Richland, WA; ²Morehouse school of medicine, Atlanta, GA; ³Department of Biochemistry and Agronomy, West Lafayette, IN; ⁴Protein Metrics, Palo Alto, CA
- WP 089 **Characterization of Hemopexin Glycosylation Associated with Liver Disease**; Miloslav Sanda; Julius Benicky; Radoslav Goldman; Georgetown University, Lombardi Cancer Center, Washington, DC
- Phosphopeptides: Enrichment Methods, 090 - 098**
- WP 090 **Fractionation Scheme Comparison for In-depth Phosphoproteome**; Qing-Run Li; Hong-Wen Zhu; Rong Zeng; Shanghai Institutes for Biological Sciences, Shanghai, China
- WP 091 **Anion-Exchange Chromatography of Tryptic Acidic Peptides and Phosphopeptides: WAX vs. SAX and AEX vs. ERLIC**; Andrew J Alpert¹; Nikolai Mischerikow²; Karl Mechtler²; ¹PolyLC Inc., Columbia, MD; ²IMP, Vienna, Austria
- WP 092 **Head-to-Head Comparison of Magnetic Beads for Phosphopeptide Enrichment**; Alex Campos; Laurence Brill; Sanford-Burnham Medical Research Institute, La Jolla, CA
- WP 093 **In-depth Characterization and Optimization of High pH Reversed-Phase Off-Line Fractionation for Phosphoproteomics**; Tanveer Batth; Chiara Francavilla; Jesper V Olsen; University of Copenhagen, Copenhagen, Denmark
- WP 094 **In vitro Evolution of DNA Aptamers Specific for the pTyr- and pSer-modified Polypeptides**; YeVa Mirzakhanyan; Jiri Misek; Andrej Luptak; Paul Gershon; UC-Irvine, Irvine, CA
- WP 095 **Everything All the Time: Comprehensive and Reproducible Phosphopeptide Enrichment using Fe³⁺ - IMAC Columns**; Benjamin Ruprecht¹; Heiner Koch¹; Max Mundt¹; Guillaume Medard¹; Bernhard Kuster¹; Simone Lemeer^{1,2}; ¹Chair of Proteomics and Bioanalytics TUM, Freising, Germany; ²Biomolecular Mass Spectrometry and Proteomics, Utrecht, Netherlands
- WP 096 **Characterization of Automated Sample Preparation Workflows Featuring Phosphopeptide Enrichment using TiO₂ Microchromatography Cartridges on a Precision Liquid Handler**; Jason Russell; Steve Murphy; Agilent Technologies, Inc., Madison, WI
- WP 097 **Thiol-phosphorylation for Monitoring Signaling to Chromatin**; Yumiao Han; Rosalynn Molden; Zuofei Yuan; Benjamin Garcia; University of Pennsylvania, Philadelphia, PA
- WP 098 **Development of a Multidimensional ERLIC/IMAC/TiO₂ Phosphoproteomic Method and Its Application to Kinase Pathway Analysis of PDGF-stimulated NIH 3T3 Cells**; Laura E. Edwards; Kevin Blackburn; Kyle G. Grant; Jason M. Haugh; Michael B. Goshe; North Carolina State University, Raleigh, NC
- Peptides: Quantitative Analysis (Applications to Peptide and Protein Targets), 099 - 121**
- WP 099 **LC-MS³ Quantitation Methods for Synthetic Glycosylated PACAP Analogs**; Nicholas Laude; Bobbi Anglin; Robin Polt; Michael Heien; University of Arizona, Tucson, AZ
- WP 100 **Quantification of Linaclotide and its Bioactive Metabolite in Human Breast Milk using LC-MS/MS**; Qingguo Tian; Andreas Grill; Daksha Desai-Krieger; Forest Laboratories, Inc., Farmingdale, NY
- WP 101 **Development of an LC-MS/MS Method for pharmacokinetic Studies of the Anticoagulant Peptide Variegins**; Norrapat Shih^{1,2}; R. Manjunatha Kini¹; ¹Dept. of Biological Sciences, National University of Singapore, Singapore; ²NUS graduate school for Integrative Sciences and, Engineering (NGS), Singapore
- WP 102 **Simultaneous Quantification of Active and Inactive Intracellular and Secreted GLP-1 Peptides from Cultured Cells by Selected Reaction Monitoring**; Michiko Amao; Yoshiro Kitahara; Ayaka Tokunaga; Kazutaka Shimbo; Yuzuru Eto; Naoyuki Yamada; Ajinomoto Co., Inc, Kawasaki-Shi, Japan
- WP 103 **A Sub-picogram (0.5 pg/ml) Level Quantification Method for Desmopressin in Human Plasma using Liquid Chromatography Electrospray Mass Spectrometry**; Rahul Baghla¹; Swati Guttikar²; Dharmesh Patel²; Abhishek Gandhi²; Anoop Kumar¹; Manoj Pillai¹; ¹AB SCIEX, Gurgaon, India; ²Veeda Clinical Research, Ahmadabad, India
- WP 104 **Quantification of Polypeptide MB56142 in Pig Lithium Heparin Plasma Using API-4000 LC-MS/MS Systems**; Guangchun Zhou; Nicole Roenker; Yong-Xi Li; Medpace, Cincinnati, OH

- WP 105 **LC/MS/MS Analysis of Active Ghrelin and the Inactive Isoform des-octanoyl-ghrelin**; David Broadwell; Derek Parks; Greg Waite; Jon D. Williams; *GlaxoSmithKline, Research Triangle Park, NC*
- WP 106 **A Rapid and Sensitive Method for the Quantification of Goserelin in Human Plasma Using HPLC-MS/MS**; Meng Fang; Yinghe Li; Yifan Shi; *Alliance Pharma, Inc, Malvern, PA*
- WP 107 **Validation of a Quantitative LC/MS/MS Method to Measure SNAP 25 Cleavage by Botulinum A Toxin**; Kathleen Housman; Joshua Emory; Nizamettin Gul; Matthew Levit; Michael Adler; Jonathan Oyler; *USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD*
- WP 108 **Quantification of Glargine and Its Metabolites in Human Plasma using a Hybrid Immunoaffinity Purification and LC-MS/MS Methodology**; Li Sun; Yang Xu; Melanie Anderson; Sheila Breidinger; Kevin Bateman; Eric Woolf; *PPDM, Merck Research Laboratories, West Point, PA*
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- WP 112 **Metallomic Analysis of Metalloproteins within the Lyme Disease Pathogen *Borrelia burgdorferi***; Matthew McIlvin¹; J. Dafne Aguirre²; Hillary Clark²; Valeria Culotta²; Mak Saito¹; ¹Woods Hole Oceanographic Inst., Woods Hole, MA; ²Johns Hopkins University, Baltimore, MD
- WP 113 **Quantification of Lysine Malonylation in SIRT5 Knockout Animals using MS1 Filtering in Skyline**; Matthew Rardin²; Yuya Nishida¹; Alexandria Sahu²; Eric Verdin²; Bradford W. Gibson²; ¹Gladstone Institute of Virology and Immunology, San Francisco, CA; ²Buck Institute for Research on Aging, Novato, CA
- WP 114 **Proteomic Analysis Defines p53 and c-myc Activities as Effective Determinants of Chronic Myeloid Leukaemia Primitive Cell Survival**; Andrew Williamson¹; Andrew Pierce¹; Lisa Hopcroft²; Sheela Abraham²; Mark Aspinall-O'Dea¹; Emma Carrick¹; Tessa Holyoake²; Anthony Whetton¹; ¹University of Manchester, Manchester, UK; ²University of Glasgow, Glasgow, UK
- WP 115 **Regulation of Protein Expression by Transcription Factors in *Saccharomyces cerevisiae***; Gennifer Merrihew; Ying Sonia Ting; Michael J. Maccoss; *University of Washington, Seattle, WA*
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- WP 117 **Proteomic Analysis of Aged *C. elegans* Infected with *P. aeruginosa***; Christina King¹; Daljeet Singh¹; Kyle Holden²; Annie Bea Govan¹; Arjumand Ghazi²; Rena A.S. Robinson¹; ¹Department of Chemistry, University of Pittsburgh, Pittsburgh, PA; ²Department of Pediatrics, Children's Hospital, Pittsburgh, PA
- WP 118 **Isolated Synaptosomes from Cortex and Striatum of Huntington Disease Mice Show Selective Loss of Synaptosome-Specific Proteins but No Bioenergetics Deficit**; Birgit Schilling; Ryan Ng; Jennifer Holcomb; Sung W. Choi; Anna Picca; Shana Katzman; Dylan J. Sorensen; Steven R. Danielson; Lisa M. Ellerby; Akos A. Gerencser; Martin D. Brand; Bradford W. Gibson; *Buck Institute for Research on Aging, Novato, CA*
- WP 119 **Kinetic Evaluation of Trypsin Digests of Apolipoprotein-A1: Implications for Quantitative Mass Spectrometry**; Scott Walmsley¹; Yuxue Liang²; Xinjian Yan²; Stephen Stein²; Alexey Nesvizhskii¹; ¹University of Michigan Department of Pathology, Ann Arbor, MI; ²NIST, Gaithersburg, MD
- WP 120 **Method Development and Validation for Multiplexing Quantitation of Proteins in Soybean Tissues Using Tandem Mass Spectrometry (LC-MS/MS)**; Ryan Hill; Trent Oman; Guomin Shan; Barry Schafer; *Dow AgroSciences, Indianapolis, IN*
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- WP 125 **Novel Integrated Microfluidics Increase Sensitivity and Reduce Sample Volume in a Quantitative LC/MS Assay for rhPTH (Teriparatide) in Human Plasma**; Erin E. Chambers^{1,2}; Mary Lame¹; Kenneth Fountain¹; ¹Waters Corporation, Milford, MA; ²King's College London, London, England
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- WP 128 **Ultra-Sensitive Quantitation of Exenatide with Micro-Flow LC Trap-and-Elute and High Resolution and Triple Quadrupole Mass Spectrometry Workflow**; Jinyuan Wang¹; Daniel Warren²; Anthony Romanelli²; ¹AB SCIEX, Redwood City, CA; ²AB SCIEX, Framingham, MA
- WP 129 **Boosting the Limits of SRM by Asn₃**; An Staes^{1,2}; Bart Ruttens^{1,2}; Luminita Moruz³; Kris Gevaert^{1,2}; ¹Department of Medical Protein Research, VIB, Gent, Belgium; ²Department of Biochemistry, Ghent University, Gent, Belgium;

- ³Department of Biochemistry and Biophysics, Stockh, Stockholm, Sweden
- WP 130 **Development of a nanoLC-MRM-based Quantitative Platform for Multiple Enzymes Associated with the Central Metabolic Pathway by using Ultra-Fast Mass Spectrometry;** Fumio Matsuda¹; Tairo Ogura²; Nobuyuki Okahashi¹; Atsumi Tomita¹; Ichiro Hirano²; Hiroshi Shimizu¹; ¹Osaka University, Suita, Japan; ²Shimadzu Corporation, Kyoto, Japan
- WP 131 **Functionalized Edman-type Reagents: Applications to Absolute Protein Quantification;** Ryo Satoh¹; Masamitsu Maekawa²; Takaaki Goto¹; Seon Hwa Lee¹; Tomoyuki Oe¹; ¹Tohoku University, Sendai, Japan; ²Tohoku University Hospital, Sendai, Japan
- WP 132 **Strategies to Eliminate Anti-Drug Antibody (ADA) Interference due to Immunogenicity on Large Molecule Quantification by LC-MS/MS;** Daniel Villeneuve; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 133 **Absolute Targeted Quantitation of Proteins and Therapeutic Biologics using Integrated LC-MS Workflow;** Xin Zhu¹; Vadi Bhat¹; Nalini Sadagopan¹; Ning Tang²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
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- WP 135 **Immobilized Monolithic Enzymatic Reactors for Online Digestion of Proteins Secreted by Developing Human Embryos;** Wei-Qiang Chen¹; Philipp Obermayr¹; Urh Černigoj³; Jana Vidič³; Miloš Barut³; Tanja Panić-Janković¹; Mikhail Gorshkov⁴; Goran Mitulović^{1,2}; ¹Medical University of Vienna, Vienna, Austria; ²Proteomics Core Facility, Medical University of Vienna, Vienna, Austria; ³BIA Separations, Ajdovščina, Slovenia; ⁴Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia
- WP 136 **Improving Prediction of IVF Success: Looking for Putative Biomarkers in IVF-Media upon Embryo Cultivation;** Tanja Panic-Jankovic³; Detlef Pietrowski¹; Weiqiang Chen³; Rainer Schmid³; Mikhail V. Gorshkov²; Anna Lobas²; Goran Mitulovic³; ¹Medizinische Universitaet Wien, Wien, Austria; ²INEPCP RAS, Moscow, Russian Federation; ³Medical University of Vienna, KIMCL, Vienna
- WP 137 **Impact of Human Blood Specimen Collection Processing, and Storage on Protein Integrity and Implications for Use in Clinical Research;** Geun-Cheol Gil; Bich Nguyen; Yiyong Zhou; Julie Lamontagne; Xiaolei Xie; Michael Schirm; Rene Allard; Daniel Chelsky; Sushmita Mimi Roy; *Caprion Proteomics US LLC, Menlo Park, CA*
- WP 138 **A Comprehensive Proteomic Study on the Effect of General Anesthesia on Human Peripheral Blood Mononuclear Cells from Colon Cancer Patients;** Xiaolei Xie; Bich Nguyen; Geun-Cheol Gil; Aude Tartiere; Louiza Mahrouche; Yiyong Zhou; Rene Allard; Daniel Chelsky; Sushmita Mimi Roy; *Caprion Proteomics US LLC, Menlo Park, CA*
- WP 139 **Integrated Approaches for Analyzing U1-70K Cleavage in Alzheimer's disease;** Bing Bai¹; Junmin Peng²; ¹Emory University, Atlanta, GA; ²St.Jude Children's Research Hospital, Memphis, TN
- WP 140 **Identification and Validation of Platelet Low Biological Variation Proteins, Superior to GAPDH, Actin and Tubulin, as Tools in Clinical Proteomics;** Marianne Koch¹; Ellen Umlauf²; Michael Veitinger²; Sheila Guterres²; Eduard Rappold⁴; Rita Babeluk²; Goran Mitulovic¹; Rudolf Oehler³; Maria Zellner²; Roland Baumgartner²; ¹Medical University of Vienna, KIMCL, Vienna, Austria; ²Med. Univ. Wien. Inst. of Physiology, Vienna, Austria; ³Med. Univ. Wien, Surgical Res. Laboratories, Vienna, Austria; ⁴Gerontology-2. Department, Otto Wagner Spital, Vienna, Austria
- WP 141 **Development and Clinical Validation of a Quantitative Mass Spectrometric Assay for PD-L1 Protein in FFPE NSCLC Samples;** Eunkyung An¹; Wei-Li Liao¹; Sheeno Thyparambil¹; Adele Blackler¹; Jaime Rodriguez²; Ravi Salgia³; Ignacio Wistuba²; Jon Burrows¹; Todd Hembrough¹; ¹OncoPlex Diagnostics, Rockville, MD; ²MD Anderson Cancer Center, Houston, TX; ³The University of Chicago, Chicago, IL
- WP 142 **Validation of Putative Proteomic Biomarkers of Clinically Significant Ureteropelvic Junction Obstruction (UPJO) via Mass Spectrometry;** John Froehlich; Richard Lee; *Children's Hospital Boston, Boston, MA*
- WP 143 **Proteomic Analysis of Biopsy Specimen Revealed the Profiles of Adenoma-Carcinoma Sequence of Colorectal Cancer;** Masaya Ono¹; Masahiro Kamita¹; Kumiko Kawasaki³; Masahiro Gomi³; Tomohiro Sakuma³; Yosuke Otake²; Taku Sakamoto²; Takeshi Nakajima²; Takahisa Matsuda²; Yutaka Saito²; Tesshi Yamada¹; ¹Natl Cancer Ctr Research Institute, Tokyo, Japan; ²Natl Cancer Ctr Hospital, Tokyo, Japan; ³Mitsui Knowledge Industry Co.,Ltd., Tokyo, Japan
- WP 144 **Designing Targeted Quantitation Methods on a Nano HPLC Q Exactive System for Proteomic Analysis of Human Pancreatic Juice;** Jenny Chen¹; Lewis Pannell²; Lindsay Schambeau²; Jana Rocker²; Gerald Concar¹; Reiko Kiyonami¹; Keith Waddell¹; ¹Thermo Scientific, San Jose, CA; ²Mitchell Cancer Institute, Mobile, AL
- WP 145 **Proteomics Analysis of Urinary Exosomes for Sensitive Detection of Tubular Injury Markers in Cystinuria;** Ida Chiara Guerrero¹; Matthieu Bourderioux¹; Cerina Chhuon¹; Thao Nguyen-khoa²; Bertrand Knebelmann²; Estelle Escudier³; Bernard Escudier⁴; Aleksander Edelman¹; ¹INSERM, Paris, France; ²APHP Necker, Paris, FR; ³APHP Trousseau, Paris, FR; ⁴Institut Gustave Roussy, Paris, FR
- WP 146 **Expression Analysis and Mass Spectrometric Structure Characterization Reveals Unknown Ezrin Truncations in Lymph Node Metastases of Breast Cancer Patients;** Claudia Röwer¹; Christian George²; Toralf Reimer²; Bernd Gerber²; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²Department of Obstetrics and Gynecology, Rostock, Germany
- WP 147 **iTRAQ-based Profiling and Label-Free Quantification Revealed a Panel of Regulated Proteins in Cervical Intraepithelial Neoplasia and Cervical Cancer Serum;** Alexander Boychenko¹; Natalia Govorukhina¹; Ate van der Zee²; Rainer Bischoff¹; ¹Analytical Biochemistry, University of Groningen, Groningen, The Netherlands; ²University Medical Centre, Groningen, The Netherlands
- WP 148 **Molecular Mechanisms of Synaptic Dysfunction in a Female Monkey Model of Depression;** Stephanie L. Willard¹; Karin E. Borgmann-Winter^{1,2}; Hoau-Yan Wang³; Matthew L. MacDonald⁴; Carol A. Shively⁵; Chang-Gyu Hahn¹; ¹University of Pennsylvania Dept of Psychiatry, Philadelphia, PA; ²Children's Hospital of Philadelphia, Philadelphia, PA; ³CUNY Medical School, Pharmacology & Neuroscience, New York, NY; ⁴University of Pittsburgh,

- Dept of Psychiatry, Pittsburgh, PA; ⁵Wake Forest School of Med, Dept of Comparative Med, Winston-Salem, NC
- WP 149 **Proteomic Analysis Reveals Defects in Energy Metabolism in Asthenozoospermia**; Guo Yueshuai; Xin Niu; Tao Zhou; Zuomin Zhou; Xuejiang Guo; Jiahao Sha; Nanjing Medical University, Nanjing, China
- WP 150 **N-terminal Proteomics using TAILS on B-lymphocytes of a Patient with Combined Immunodeficiency**; Theo Klein¹; Shan-Yu Fung^{1,2}; Michael A. Blank³; Rosa Viner³; Stuart Turvey^{1,2}; Christopher M. Overall¹; ¹UBC, Vancouver, Canada; ²Children and Family Research Institute, Vancouver, Canada; ³Thermo Fisher Scientific, San Jose, CA
- WP 151 **A Novel LC-MS Method for the Detection of Mutations Related to Antibiotic Resistance in Gyrase of Salmonella Isolates**; Lennard Dekker; Robbert-Jan Hassing; Lona Zeneyedpour; Theo Luiders; Wil Goessens; Erasmus Medical Center, Rotterdam, The Netherlands
- WP 152 **Integration of SWATH and MRM for Biomarker Discovery of Esophageal Squamous Cell Carcinoma**; Guixue Hou^{1,2}; Liang Lin²; Xiaomin Lou¹; Jin Zi²; Quanhui Wang^{1,2}; Yulin Sun³; Xiaohang Zhao³; Siqi Liu^{1,2}; ¹Beijing Institute of Genomics, CAS, Beijing, China; ²BGI-Shenzhen, Shenzhen, China; ³Cancer Institute, CAMS, Beijing, China
- WP 153 **Analysis of Surface Charge Influences in Interactions of Nanoparticles with Human-Bronchoalveolar-Lavage-Fluid using HPLC - MS/MS**; Theresa Kristl¹; Matthew Boyles¹; Martin Himly¹; Romana Mikes²; Michael Studnicka²; Albert Duschl¹; Christian Huber¹; ¹University of Salzburg, Salzburg, Austria; ²Paracelsus Medical University, Salzburg, Austria
- WP 154 **Evaluation of Targeted Proteomics Approaches for Optimal Quantification Strategies Applied to Drug Toxicity Profiling in 3D Tissue Models**; Asa Wahlander¹; Nathalie Selevsek¹; Jonas Grossmann¹; Christian Panse¹; Patrina Gunness²; Jens Kelm²; Ralph Schlapbach¹; ¹Functional Genomics Center Zurich (FGCZ), Zurich, Switzerland; ²InSphero AG, Schlieren, Switzerland
- WP 155 **A Rapid, Data Independent Acquisition Method for Population-Scale Proteome Barcoding using PCT-SWATH**; Tiannan Guo; Ruedi Aebersold; ETH Zurich, Zurich, Switzerland
- WP 156 **Automated Top-Down Mass Spectrometry of Hemoglobin for a Clinical Application**; Didia Coelho Graça¹; Adelina E Acosta-Martin^{1,2}; Wolfgang Jabs³; Ralf Hartmer³; Lorella Clerici²; Markus Meyer³; Kaveh Samii⁴; Yury O Tsybin⁵; Denis Hochstrasser^{1,2}; Pierre Lescuyer^{1,2}; Alexander Scherl^{1,2}; ¹DHPS, Faculty of Medicine, Geneva University, Geneva, Switzerland; ²DGLM, Geneva University Hospitals, Geneva, Switzerland; ³Bruker Daltonics, Bremen, Germany; ⁴Division of Hematology, Geneva University Hospital, Geneva, Switzerland; ⁵BMSL, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- WP 157 **Label-Free Quantitation of Proteoforms by High-Throughput Top Down Proteomics for Biomarker Discovery**; Ioanna Ntai¹; Kyung-Kon Kim¹; Ryan Fellers¹; Owen Skinner¹; Bryan Early¹; Richard Leduc²; Paul Thomas¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Indiana University, Bloomington, IN
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- WP 158 **Description of a Novel Multi-Column / Multi-Dimensional nanoLC-MS/MS Platform for Automated Proteomic Analysis**; Steven Mullett¹; Gary Valaskovic²; Mike Lee³; Nathan Yates¹; ¹University of Pittsburgh, Pittsburgh, PA; ²New Objective, Inc., Woburn, MA; ³Milestone Development Services, Newtown, PA
- WP 159 **The Integration of Nano Scale Separation and Ionization for the Analysis of Complex Proteomes**; Peter Wang¹; Zhou Hu²; Yang Yi-Ming²; Amanda Berg³; Gary A. Valaskovic³; ¹New Objective, Inc., Shanghai, China; ²Shanghai Institute of Materia Medica, CAS, Shanghai, China; ³New Objective, Inc., Woburn, MA
- WP 160 **Comparison of Shotgun Proteomic Methods For Small Scale Analysis of Complex Proteomes**; Lu Yu; Jyoti Choudhary; Wellcome Trust Sanger Institute, Cambridge, UK
- WP 161 **Online Affinity and Digestion: A Flexible and Robust Tool for the Characterization and Quantification of Proteins**; David Colquhoun¹; Mohamed Nazim Boutaghou¹; Rachel Lieberman¹; Brian Feild¹; Kevin W. Meyer²; Scott Kuzdzal¹; ¹Shimadzu Scientific Instruments, Columbia, MD; ²Perfinity Biosciences, West Lafayette, IN
- WP 162 **Investigation of Fractionation Strategies for Intact Proteins Compatible with Top-down Mass Spectrometry**; Santosh G. Valeja¹; Lichen Xiu²; Andrew J. Alpert³; Song Jin²; Ying Ge^{1,2}; ¹Dept. of Cell & Regenerative Biology, UW-Madison, Madison, WI; ²Department of Chemistry, UW-Madison, Madison, WI; ³PolyLC Inc., Columbia, MD
- WP 163 **Fluorescence Complementation - Mass Spectrometry (FC-MS) for Identifying Direct Upstream Kinases**; Lingfei Zeng¹; Chang-Deng Hu¹; Weiguo Tao²; ¹Department of MCMP, Purdue University, West Lafayette, IN; ²Department of Biochemistry, Purdue University, West Lafayette, IN
- WP 164 **Applicability of Partial Edman Degradation for MS/MS-free Protein Identifications in Shotgun Proteomics**; Anna A. Lobas¹; Mark V. Ivanov¹; Lev I. Levitsky¹; Marina L. Pridatchenko¹; Irina A. Tarasova¹; Alexander V. Gorshkov²; Anatoly N. Verenchikov³; Mikhail V. Gorshkov¹; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russia; ²N.N. Semenov's Institute of Chemical Physics, Moscow, Russia; ³Mass Spectrometry Consulting Ltd., Bar, Montenegro
- WP 165 **Isolation of N-terminal Fragments from Cyanogen Bromide Cleaved Proteins after Combined Micro Liquid- and Solid Phase Derivatization**; Heinz Nika¹; David Hawke²; Ruth Hogue Angeletti¹; ¹Albert Einstein College of Medicine, Bronx, NY; ²UT- M.D. Anderson Cancer Center, Houston, TX
- WP 166 **Dual Matrix-Based Immobilized Trypsin Combined magnetic Separation for Fast Proteolytic Digestion and In-depth Proteomics Analysis**; Wanjun Zhang; Chao Fan; Duan Feng; Weijie Qin; Xiaohong Qian; Beijing Proteome Reserach Center, Beijing, China
- WP 167 **A New Protease for Bottom Up and Middle-Down Proteomics**; Martial Rey¹; Hynek Mrazek²; Petr Halada²; Petr Man²; David Schriemer¹; ¹University of Calgary, Calgary, Canada; ²Institute of Microbiology, Prague, Czech Republic
- WP 168 **Amino Acid Labeling With Tryptic Digestion: An Approach for Middle-Down Proteomics**; Nathanael F. Zinnel; William K. Russell; David H. Russell; Texas A&M University, College Station, TX
- WP 169 **Introducing a Highly Selective Cleavage into Proteins in a Pseudo-Top Down Proteomics Approach to Produce Simplified and Predictable Fragmentation Spectra**; William Mcgee¹; Zhen Wu¹; Victoria Hedrick²; Lake Paul²; Mary Wirth¹; Scott McLuckey¹; ¹Purdue University, West Lafayette, IN; ²Purdue Proteomics Facility, West Lafayette, IN

- WP 170 **A Thermostable, N-terminal Arginine and Lysine Specific Protease for ≤ 1 hr Digestion, Simplified Peptide Fragmentation and Increased MS/MS Sensitivity**; John P. Wilson¹; Jonathan J. Ipsaro¹; Samantha N. Peacock¹; Keith D. Rivera¹; Katharine H. Dusenbury²; Darryl J.C. Pappin¹; ¹Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; ²Dana Farber Cancer Institute, Boston, MA
- WP 171 **Chemical Cleavage for Middle-Down Analysis by Electron Transfer Dissociation**; Jan Fish; Jasparl Cheema; Elzbieta Piatkowska; Sarah R Hart; Keele University, Newcastle-Under-Lyme, UK
- WP 172 **Chemical Hydrolysis-Based Middle-Down Proteomics**; Kristina Srzentić¹; Grigory Karateev¹; Luca Fornelli¹; Lev I. Levitsky²; Anna A. Lobas²; Elena Dubikovskaya¹; Mikhail V. Gorskhov²; Unige A. Laskay¹; Daniel Ayoub¹; Yury O. Tsybin¹; ¹Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia
- WP 173 **N-terminal Positional Proteomics using SPITC (4-sulfophenyl isothiocyanate) for Enrichment and Identification**; Yanjie Jiang^{1,2}; James Madsen¹; Victor Farutin¹; Jonathan Lansing¹; Richard Cole^{2,3}; ¹Momenta pharmaceuticals, Cambridge, MA; ²Department of Chemistry, University of New Orleans, New Orleans, LA; ³Université Pierre et Marie Curie, Paris, France
- WP 174 **Automated Protein Digestion Workflows for MS-based Proteomics Applications**; Gunnar Dittmar¹; Oliver Popp¹; Guenter Boehm²; Andreas Bruchmann³; ¹MDC, Berlin, Germany; ²CTC Analytics, Zwingen, Switzerland; ³Axel Semrau GmbH, Sprockhovel, Germany
- WP 175 **Optimization of Dual Polarity Ultraviolet Photodissociation Proteomics**; Sylvester Greer; Jennifer Brodbelt; The University of Texas, Austin, TX
- WP 176 **Higher Confidence Analysis of E. coli Lysate by Reducing Spectral Complexity Using 351 nm UVPD**; Scott Robotham; Joe Cannon; Jennifer Brodbelt; University of Texas at Austin, Austin, TX
- WP 177 **Specific Detection of Proteins in Biological Matrices by Targeting Cysteine-Containing Peptides with Visible Photodissociation in an Q-Exactive Mass Spectrometer**; Marion Girod; Jordane Biarc; Rodolphe Antoine; Philippe Dugourd; Jérôme Lemoine; University of Lyon, Villeurbanne, France
- WP 178 **Towards Cell-Type Specific Nuclear Proteomes from Human Neurodegenerative Disease Brain**; Eric Dammer; Duc Duong; Ian Diner; James Lah; Allan Levey; Nicholas Seyfried; Emory University, Atlanta, GA
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- WP 179 **Internal Standardization Approaches for Quantification of 25k Da Fusion Protein to Support Early Stage Drug Development by LC-MS**; Jean-Nicholas Mess¹; Karl-Rudolf Erlemann²; Jerzy Pieczykolan³; Sebastian Pawlak³; Fabio Garofolo¹; ¹Algorithme Pharma Inc., Laval, QC, Canada; ²InSymbiosis, Montreal, QC, Canada; ³Adamed Group, Czosnow, Poland
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- WP 182 **Analysis of Polysorbates in Biotherapeutic Products using Two-Dimensional HPLC Coupled with Mass Spectrometer**; William Hedgepeth; Kenichiro Tanaka; Shimadzu Scientific Instruments, Inc., Columbia, MD
- WP 183 **A Versatile Method using Immunoaffinity LC-MS/MS to Quantify Antigen Protein in Animal Studies of Monoclonal Antibody Therapeutics**; Ichiro Onami; Miho Ayabe; Naoaki Murao; Masaki Ishigai; Chugai Pharmaceutical Company, Ltd., Gotemba, Japan
- WP 184 **LC-MS Method Development for Therapeutic Antibody Quantitation in Animal Plasma**; Qian Zhang¹; Zhenlian Ke¹; Daniel Spellman¹; Nathan Hatcher¹; Daniela Tomazela²; Maribel Beaumont²; Bernard Choi³; Jane Harrelson¹; Kevin Bateman¹; ¹Merck & Co., Inc., West Point, PA; ²Merck & Co., Inc., Palo Alto, CA; ³Merck & Co., Inc., Rahway, NJ
- WP 185 **The Optimization of Host-cell Protein Detection using Data-Independent SWATH-MS**; Randy J. Arnold; Eric Johansen; Justin Blethrow; AB Sciex, Redwood City, CA
- WP 186 **Automated High Throughput Peptide and Protein MRM Optimization for Pharmaceutical Method Development**; Ian Moore; Suma Ramagiri; AB SCIEX, Concord, Canada
- WP 187 **Quantitative Proteomic Analysis of Outer Membrane Vesicles (OMV) from Neisseria meningitidis**; Alessandro Vadi; Novartis Vaccines and Diagnostics, Siena, IT
- WP 188 **Method Validation and Sample Analysis of a Protein Drug Candidate in Monkey Serum Using LC-MS/MS**; yue zhao; Guowen Liu; aida angeles; Lora Hamuro; mark arnold; jim shen; Bristol-Myers Squibb Co., Princeton, NJ
- WP 189 **Relative Quantification of MABS Glycosylation Changes during Stability and Accelerated Degradation Studies using Stable-Isotope Labeling and UPLC-ESI-QTOF**; Silvia Millan Martin¹; Cedric Delporte¹; Natalia Navas²; Niaobh McLoughlin¹; Jonathan Bones¹; ¹NIBRT, Dublin, Ireland; ²UGR (University of Granada), Granada, Spain
- WP 190 **Development of a High Resolution LC-MS Method for Absolute Quantitation of Hemagglutinin and Neuraminidase Proteins in Influenza Virus-Like Particle Vaccines**; Jingzhong (Tim) Guo; Yali Lu; Jingning Li; Ziping Wei; Erica Shane; Oleg Borisov; NovaVax, Rockville, Md
- WP 191 **A Streamlined Workflow for Characterizing Low Abundance Glycans on Therapeutic Proteins**; Michael Kimzey; Shiva Pourkaveh; Samnang Tep; Sybil Lockhart; Justin Hyche; Ted Haxo; Jo Wegstein; ProZyme, Hayward, CA
- WP 192 **A Simple and Robust Targeted Quantitative Method for Insulin and its Therapeutic Analogs**; Eric Niederkofler¹; Scott Peterman²; Amanda Leber¹; Kwasi Antwi¹; Tara Schroeder²; Urban Kiernan¹; Kemmons Tubbs¹; Bryan Krastins²; Amol Prakash²; Jennifer L. Frahm³; Mary F Lopez²; ¹Thermo Fisher Scientific, Tempe, AZ; ²Thermo Fisher Scientific, BRIMS, Cambridge, MA; ³Thermo Fisher Scientific, San Diego, CA
- WP 193 **Surfactant-aided Precipitation/On-Pellet-Digestion (SOD) for Straightforward, Efficient and Reproducible Sample Preparation for Targeted Quantification of mAb in Plasma and Tissues**; Bo An^{1,2}; Ming Zhang^{1,2}; Jun Qu^{1,2}; ¹SUNY at Buffalo, Buffalo, NY; ²New York State Center of Excellence, Buffalo, NY, Buffalo, NY
- WP 194 **Direct Analysis of Cell Culture Media using Targeted Peptide Mapping to Analyze the Post-Translational Modifications of Recombinant Proteins**; Chris Barton; Jeong Lee; Xiaojun Lu; David Spencer; Mark Schenerman; Jihong Wang; MedImmune, Gaithersburg, MD
- WP 195 **Multiplex Quantitation of Reversible Cysteine Oxidation in Mouse Heart: Effects of Catalase Overexpression and Type-2 Diabetogenic Diet**; Chunxiang Yao; Jessica



- Behring; Deborah Siwik; Stephen Whelan; Catherine E. Costello; Wilson Colucci; Richard Cohen; Mark E. McComb; Markus Bachschmid; *Boston University School of Medicine, Boston, Ma*
- WP 196 **MS in QC: A Fully Compliant Multi-Attribute Quantitative Method for Quality Control and Release Testing of Biologics;** Sabrina Benchaar¹; Richard Rogers²; Nancy Nightlinger²; Quanzhou Luo¹; Amanda Miller²; Wenzhou Li¹; Brittney Livingston²; Gang Huang¹; Robert Bailey²; Ryo Komatsuzaki³; Jennifer Sutton³; Christoph Nickel³; Alain Balland²; ¹*Amgen, Thousand Oaks, CA*; ²*Amgen, Seattle, WA*; ³*ThermoFisher Scientific, San Jose, CA*
- WP 197 **Release Testing of Biotherapeutics by Mass Spectrometry with Automated Detection of Unexpected Features;** Richard Rogers¹; Nancy Nightlinger¹; Jennifer Sutton²; Sabrina Benchaar³; Alain Balland¹; Robert Bailey¹; ¹*Amgen, Seattle, WA*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*Amgen, Thousand Oaks, CA*
- WP 198 **The Effects of Alternative Carbon Sources on CHO Cell Metabolism and Product Quality;** Peter Slade¹; Guy Caspary¹; Shilpa Nargund²; Arvia Morris¹; ¹*Amgen, Seattle, WA*; ²*Amgen, Thousand Oaks, CA*
- WP 199 **Evaluation of Label-free MS-based Relative Quantitation of Post-translational Modifications of Therapeutic proteins;** Hongji Liu; Qing Paula Lei; Michael Washabaugh; *MedImmune, Gaithersburg, MD*
- WP 200 **High Throughput Screening of Deubiquitylase Activity, Specificity and Inhibition by MALDI-TOF Mass Spectrometry;** Maria Stella Ritorto¹; Richard Ewan¹; Ana Perez-Oliva¹; Axel Knebel¹; Nicholas Morrice²; Dario Alessi¹; Matthias Trost¹; ¹*MRC Protein Phosphorylation and Ubiquitylation Uni, Dundee, UK*; ²*The Beatson Institute for Cancer Research, Glasgow, UK*
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- WP 205 **Reducing Time-to-Measurement of Monoclonal Antibodies Using Microfluidic LC/MS Approaches;** Gregory Staples; Hongfeng Yin; Kevin Killeen; *Agilent Laboratories, Santa Clara, CA*
- WP 206 **Variant Identification from Human Recombinant Erythropoietin by LC-MS/MS;** Jung-Keun Suh¹; Hyong-Ha Kim²; ¹*Korean German Institute of Technology, Seoul, South Korea*; ²*Korea Research Institute of Standards and Science, Daejeon, Korea*
- WP 207 **Novel Protein Targets of Indomethacin in BT474 Human Breast Cancer Cells using Proteomics;** Valeriy Shevchenko; Sergei Kovalev; Marat Taipov; Natalia Arnotskaya; Igor Kudryavtsev; *N. N. Blokhin Russian Cancer Research Center, Moscow, Russian Federation*
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- WP 218 **The Combination of Molecular Dynamics, Amide Hydrogen Exchange, and Mass Spectrometry to Understand mAb Conformational Dynamics;** Benjamin Walters¹; Thomas Patapoff²; Jennifer Zhang¹; ¹*Protein Analytical Chemistry, Genentech Inc., South San Francisco, CA*; ²*Early Stage Pharmaceutical Dev., Genentech Inc., South San Francisco, CA*
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- WP 220 **Dynamics of the SH3 Domains of Tec Family Tyrosine Kinases by Hydrogen Exchange Mass Spectrometry;** Justin Roberts¹; Sreya Tarafdar²; Thomas Wales¹; Thomas Smithgall²; John Engen¹; ¹Northeastern University, Boston, MA; ²University of Pittsburgh, Pittsburgh, PA
- WP 221 **Probing Regulatory Domain Interactions in the Tec-family Tyrosine Kinase Btk using HXMS;** Thomas E. Wales¹; Raji E. Joseph²; Amy H. Andreotti²; John R. Engen¹; ¹Northeastern University, Boston, MA; ²Iowa State University, Ames, IA
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- WP 225 **Structural and Functional Insights of Small Molecule Disruptors of the Glucokinase-Glucokinase Regulatory Protein Interaction by Hydrogen/Deuterium Exchange Mass Spectrometry;** Min Shen; Klaus Michelsen; Paul Schnier; *Amgen Inc., Thousand Oaks, CA*
- WP 226 **Probing the Conformational Dynamics of a Novel Kinase Induced by ATP and Substrate Binding by HDX-MS;** Jianzhong Wen¹; Sheng Li²; Jeffrey Esko¹; Jack E. Dixon¹; ¹UC San Diego, San Diego, CA; ²UCSD, La Jolla, CA
- WP 227 **Congo Red Induced Unfolding of Human Insulin by Pulsed Labeling Hydrogen-Deuterium Exchange Coupled with ESI and Mass Spectrometry;** Teerapat Rojsajjakul; Fred King; *Department of Chemistry, West Virginia University, Morgantown, WV*
- WP 228 **Structural Characterization of Hsp70 Protein Complexes using Hydrogen Deuterium Exchange Mass Spectrometry;** Victoria A. Assimon¹; Jennifer N. Rauch¹; Terry Zhang²; Shenheng Guan¹; Jason E. Gestwicki¹; ¹Institute for Neurodegenerative Diseases, San Francisco, CA; ²Thermo Fisher Scientific, San Jose, CA
- WP 229 **The Non-Native Code of Secreted Preproteins Investigated by HDX-MS and Native IM/MS;** Alexandra Tsirigotaki^{1,2}; M. Papanastasiou³; A. Konijnenberg⁴; K. Chatzi¹; M.B. Trelle⁵; T.J.D. Jørgensen⁵; F. Sobott⁴; S. Karamanou^{1,3}; A. Economou^{1,2}; ¹Dpt of Microbiology and Immunology, KU Leuven, Leuven, Belgium; ²IMBB, FoRTH, Dpt of Biology, UoC, Iraklio, Crete, Greece; ³IMBB, Forth, Iraklio, Crete, Greece; ⁴Chemistry Department, U. Antwerpen, Antwerp, Belgium; ⁵Dpt of Biochemistry and Molecular Biology, SDU, Odense, Denmark
- WP 230 **Allosteric Conformational Destabilization of CFTR Nucleotide Binding Domain 1 (NBD1) by the Cystic Fibrosis Mutation $\Delta F508$;** Naoto Soya^{1,2}; Ariel Roldan¹; Miklos Bagdany¹; Gergely Lukacs^{1,2}; ¹Department of Physiology, McGill University, Montreal, Canada; ²GRASP, McGill University, Montreal, Canada
- WP 231 **HDX and MS Reveals pH-dependent Conformational Changes of Monomeric and Dimeric Diphtheria Toxin T Domain;** Jing Li¹; Mykola Rodnin²; Alexey Ladokhin²; Michael Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²University of Kansas Medical Center, Kansas City, KS
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- WP 233 **Quantitative Proteomics of Estrogenic Effects in the Rat Uterus in vivo;** Fatima Sahyouni; Szabolcs Szarka; Vien Nguyen; Katalin Prokai-Tatrai; Laszlo Prokai; *University of North Texas Health Science Center, Fort Worth, TX*
- WP 234 **Quantitative Proteomic Analysis of Rat Adrenal Medulla in Response to 2-deoxy-D-glucose;** Mehdi Mirzaei¹; Masoud Zabet Moghaddam²; Lindsay Parker¹; Phill Bokiniac¹; Yunqi Wu¹; Paul Haynes¹; Ann Goodchild¹; ¹Macquarie University, Sydney, Australia; ²Texas Tech University, Lubbock, TX
- WP 235 **Quantitative Proteomic Analysis of Various Grades of Glioma Tissues Across Indian Patient Population;** Kishore Gollapalli²; Ravi Kumar Krovvidi¹; Leo Bonilla¹; sanjeeva Srivastava²; ¹Agilent Tech, Richland, WA; ²Dept of Biosciences and Bioengineering, Mumbai, India
- WP 236 **High Pressure-Assisted Extraction for the Improved Proteomic Analysis of FFPE Tissue;** Carol B. Fowler¹; Timothy J. Waybright²; Timothy D. Veenstra²; Timothy J. O'Leary³; Jeffrey T. Mason¹; ¹Baltimore VA Medical Center, Baltimore, MD; ²National Cancer Institute, Frederick, MD; ³BLR&D Service, Veterans Health Administration, Washington, DC
- WP 237 **Evaluating the Effect of Formalin Fixation on Mass Spectrometry Based Proteomic Profiling;** Drexel Neumann¹; Eric Dammer²; Duc Duong²; Nicholas Seyfried²; James A Atwood¹; ¹Omni International, Inc., Kennesaw, GA; ²Emory University, Atlanta, GA
- WP 238 **A Novel Approach for the Analysis of Membrane Proteins Applied to Glioma Stem Cell Xenografts;** Norelle Wildburger¹; Cheryl Lichti¹; Ekaterina Mostovenko¹; Frederick Lang²; Joy Gumin²; Carol Nilsson¹; ¹UTMB, Galveston, TX; ²MD Anderson Cancer Center, Houston, TX
- WP 239 **Proteomics Analysis of Decellularized Biological Scaffolds for Tissue Engineering;** Qiyao Li¹; Changying Ling²; Sinan Ozer^{3,4}; Brian Frey¹; Zhen Chang²; Basak Uygun^{3,4}; Nathan Welham²; Lloyd Smith¹; ¹Dept. of Chemistry, UW-Madison, Madison, WI; ²Dept. of Surgery, UW-Madison, Madison, WI; ³Center for Engineering in Medicine, Boston, MA; ⁴Massachusetts General Hospital, Boston, MA
- WP 240 **A Proteomic Profiling Strategy for the Non-Human Primate Animal Model, Rhesus Monkey;** Jin-Gyun Lee¹; Kimberly McKinney¹; Yong-Yook Lee¹; Haena Chung¹; Antonis Pavlopoulos¹; Kook Jung¹; Woong-Ki Kim²; Marcelo Kuroda³; Sunil Hwang¹; ¹Carolinas Healthcare System, Charlotte, NC; ²Eastern Virginia Medical School, Norfolk, VA; ³Tulane University, Covington, LA
- WP 241 **Large Scale Kinome Analysis of Human Skeletal Muscle using ATP Probes and HPLC-ESI-MS/MS;** Yue Qi; Danjun Ma; Michael Caruso; Monique Lewis; Xiangmin Zhang; Wissam Al-Janabi; Divyasri Damacharla; Zhao Yang;

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- WP 243 **Quantitative Proteomic and Systems Analysis of Cells in Response to External Stimuli;** Allison Galassie¹; Parimal Samir²; Kristen Hoek²; Xinnan Niu²; Andrew Link²; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt University School of Medicine, Nashville, TN
- WP 244 **Tracking the Impact of Viral Infection on Cellular Organelle Remodeling using Quantitative Organelle Proteomics;** Pierre Jean Beltran; Rommel Mathias; Todd M. Greco; Ileana M. Cristea; Princeton University, Princeton, NJ
- WP 245 **Uncovering Cytomegalovirus-Targeted Host Cellular Processes by Quantifying Changes in the Nuclear Proteome;** Dominique Carter^{1,2}; Justin Reitsma^{1,2}; Kathleen Noon^{1,3}; Scott Terhune^{1,2}; ¹Medical College of Wisconsin, Milwaukee, Wisconsin; ²Microbiology & Molecular Genetics, Milwaukee, WI ³Biotechnology & Bioengineering Center, Milwaukee, WI
- WP 246 **Quantitative Proteomics of MAOA-knockdown Prostate Cancer Cells;** Sheng-Ta Tsai¹; Shok-Li Ng¹; Kai-Yun Chen¹; Ting-Jen Cheng¹; Jason Boyang Wu²; Jean Chen Shih³; Chung-Hsuan Chen¹; ¹Genomics Research Center, Taipei, Taiwan; ²Cedars-Sinai Medical Center, Los Angeles, CA; ³University of Southern California, Los Angeles, CA
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- WP 248 **Skin Aging – Identification of Proteins Related to *in situ* Aging of Human Dermal Fibroblasts using a Quantitative Proteomic Approach;** Daniel M. Waldera-Lupa¹; Faiza Khalfallah²; Fritz Boege²; Kai Stühler¹; ¹Molecular Proteomics Laboratory, Düsseldorf, Germany; ²Zentralinstitut für Klinische Chemie, Düsseldorf, Germany
- WP 249 **Proteomic Analysis of Adipocytes in Response to Fructose and Glucose Treatment;** Yuan Gao; Vijayalakshmi Varma; Greg T. Nolen; Zhijun Cao; Li-Rong Yu; National Center for Toxicological Research, FDA, Jefferson, AR
- WP 250 **Elucidating Global Proteomic Changes Induced by the Epstein-Barr Virus Oncoproteins LMP1 and LMP2A;** Robert M. DeKroon¹; Harsha P. Gunawardena²; Nancy Raab-Traub¹; ¹Lineberger Comprehensive Cancer Center, UNC-Chapel Hill, NC; ²Program in Molecular Biology & Biotechnology, UNC-Chapel Hill, NC
- WP 251 **Insights into Kinome Perturbation during NLRP3 Inflammasome Activation using an Isotope-Coded ATP-affinity Probe and Targeted Mass Spectrometry;** Preston Williams; Lei Guo; Yinsheng Wang; University of California - Riverside, Riverside, CA
- WP 252 **Label-free Quantitative Proteomics Study of the Synergistic Effect of Oxacillin and a Novel Erythromycin Derivative against Methicillin-Resistant *Staphylococcus aureus*;** Xiaofen Liu¹; Pei-Jing Pai¹; Yingwei Hu¹; Daijie Chen²; Henry Lam¹; ¹Hong Kong University of Science and Technology, Hong Kong, China; ²China State Institute of Pharmaceutical Industry, Shanghai, China
- WP 253 **Interactome of a Jumping Gene;** Martin S. Taylor¹; John LaCava²; Paolo Mita¹; Kelly R. Molloy²; Donghui Li¹; Emily M. Adney¹; Hua Jiang²; Brian T. Chait²; Michael P. Rout²; Jef D. Boeke³; Lixin Dai¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD; ²The Rockefeller University, New York, NY; ³NYU Langone University School of Medicine, New York, NY
- WP 254 **Proteomics Methods for Chinese Hamster Ovary (CHO) Cell Culture Optimization;** Gang Xiao; Sohye Kang; Pavel Bondarenko; Da Ren; Amgen Inc., Thousand Oaks, CA
- WP 255 **Proteomic Investigation of the Osmoregulatory Protein Interactome using the Mass Spectrometry-Cleavable Chemical Crosslinker DC4;** Kevin R. Ramkissoon¹; Jenna F. Dumond¹; Guanghui Wang²; Marjan Gucek²; Maurice B. Burg¹; Joan D. Ferraris¹; ¹Systems Biology Center, NHLBI, NIH, Bethesda, MD; ²Proteomics Core, NHLBI, NIH, Bethesda, MD
- WP 256 **Proteomic Profiling of the Secretome upon Toll-like Receptor Stimulation;** Marijke Koppenol-Raab; Virginie Sjoelund; Aleksandra Nita-Lazar; NIH/NIAID/LSB, Bethesda, MD
- WP 257 **In-depth and Time-Resolved Dissection of Early Phosphoproteome and Ensuing Proteome Changes in Response to TGF- β ;** Kirti Sharma¹; Rochelle CJ D'souza¹; Anna Korhonen^{2,4}; Nagarjuna Nagaraj¹; Chunaram Choudhary³; Peter ten Dijke²; Matthias Mann^{1,3}; ¹Max Planck Institute for Biochemistry, Martinsried (Near Munich), Germany; ²Leiden University Medical Center, Leiden, The Netherlands; ³University of Copenhagen, Copenhagen, Denmark; ⁴University of Turku, Turku, Finland
- WP 258 **Filamentous Growth Response of Yeast by Quantitative Phosphoproteomics;** Hye Kyong Kweon; Christian Shively; Anuj Kumar; Philip Andrews; The University of Michigan, Ann Arbor, MI
- WP 259 **Quantitative Analysis of HDAC6-regulated Proteome and Lys Acetylome;** Yue Chen¹; Zhongyi Cheng¹; Rui Hao²; Sangkyu Lee¹; Tso-Pang Yao²; Yingming Zhao¹; ¹University of Chicago, Chicago, IL; ²Duke University, Durham, NC

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- WP 265 **Monoclonal Antibody and Related Product Characterization under Native Conditions using a Benchtop Exactive Plus EMR Mass Spectrometer;** Yue Xuan¹; Francois Debaene²; Johann Stojko²; Alain Beck³; Alain Van Dorsselaer²; Sarah Cianferani²; Maciej Bromirski¹; ¹Thermo Fisher Scientific GmbH, Bremen, Germany; ²University of Strasbourg, Strasbourg, France; ³Pierr-Fabre, Strasbourg, France
- WP 266 **Highly Sensitive and Robust LC-MS Method for Therapeutic Monoclonal Antibody Analysis from Complex Matrices;** Joshua Nicklay¹; Eric Niederkofler²; Urban Kiernan²; Kemmons Tubbs²; Scott Peterman³; ¹Thermo Fisher Scientific, Somerset, NJ; ²Thermo Fisher Scientific, Tempe, AZ; ³Thermo Fisher Scientific BRIMS, Cambridge, MA
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- WP 268 **Liquid Chromatography-High Resolution Mass Spectrometry Bioanalytical Approach for the Quantification of Total Antibody-Drug Conjugate (ADC, DAR \geq 0) in Rat Plasma;** Jean-Nicholas Mess¹; Suma Ramagiri²; Gary Impey²; Fabio Garofolo¹; *Algorithme Pharma Inc., Laval, Quebec, Canada; ²AB Sciex, Concord, Ontario, Canada*
- WP 269 **Intact Protein Separation by CE-UV/MALDI-MS for Top-Down Proteomics;** Michael Biacchi¹; Alain Beck²; Yannis Francois¹; Emmanuelle Leize-Wagner¹; ¹LSMIS UMR-CNRS7140, University of Strasbourg, Strasbourg, France; ²Centre d'immunologie Pierre Fabre, Saint-Julien en Genevois, Francois
- WP 270 **Accurate Identification of Drug Conjugation Sites on Antibody-Drug Conjugates using MS/MS;** Kelli Jonakin; Eric Johansen; St John Skilton; Justin Blethrow; *AB SCIEX, Redwood Shores, CA*
- WP 271 **Optimizing Chromatography and High Resolution Time-of-Flight Mass Spectrometry for Antibody-Drug Conjugate DAR Characterization;** Katherine Wright¹; Shakey Quazi¹; Brigitte Simons²; Dawn Dufield¹; ¹Pfizer, Andover, MA; ²AB SCIEX, Concord, ON
- WP 272 **Direct Measurement of Conjugated Drug on ADC with Cleavable Linker via Enzymatic Cleavage and LC/MS Analysis;** Brian Rago¹; Sean Han¹; Frank Barletta²; ¹Pfizer, Groton, CT; ²Pfizer, Pearl River, NY
- WP 273 **Overcoming Challenges in Heightened Characterization for Antibody Drug Conjugates with Unique Approaches, New Methodologies and Ultrahigh-Resolution Mass Spectrometry;** Olga Friese¹; Jacquelyn Smith¹; James Carroll¹; Jason Rouse²; ¹Pfizer, Inc., St. Louis, MO; ²Pfizer, Inc, Andover, MA
- WP 274 **Characterization of Isoforms of Cysteine-Conjugated Antibody Drug Conjugates (ADCs) using On-line 2D-LC/MS;** Frank Kotch¹; Robert Birdsall²; Henry Shion²; April Xu¹; Thomas Porter³; Weibin Chen²; ¹Pfizer, Pearl River, NY; ²Waters Corporation, Milford, MA; ³Pfizer, Andover, MA
- WP 275 **Rapid Mass Analysis of the Minor Variants in IgG1 Antibodies by 2D-LC/Q Exactive System;** Jin Li; *Genentech, South San Francisco, CA*
- WP 276 **Rapidly Quantify Tryptophan Oxidation of an IgG1 Antibody Fragment by Parallel-Reaction-Monitoring Based HR/AM Approach on an UHPLC/Q Exactive System;** Weitao Jia; Jennifer Zhang; *Genentech Inc., South San Francisco, CA*
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- WP 280 **Analysis of Lipids in Serum Using Continuous Tandem Spectra Acquisition and Customized Instrument Control Software;** Joseph A. Hankin¹; Robert M. Barkley¹; Jeff Brown²; Mike Morris²; Emmy Hoyes²; Richard Chapman²; Robert Murphy¹; ¹University of Colorado Denver, Aurora, CO; ²Waters Corporation, Manchester, UK
- WP 281 **Plasma Lipid Profiling using high Resolution Mass Spectrometry and Complementary Fragmentation Strategies;** Claire Dauly¹; Alexandre Seyer²; Samia Boudah³; Simon Broudin²; Christophe Junot³; Benoit Colsch³; ¹Thermo Fisher Scientific, Courtaboeuf, France; ²Profilomic SA, Boulogne-Billancourt, France; ³CEA-Centre d'Etude de Saclay, Laboratoire d'étud, Gif-sur-Yvette, France
- WP 282 **Systematic Characterization of Experimental Conditions for High-Throughput Yeast Lipid Profiling by MALDI-MS;** Junya Nakamura¹; Daichi Yukihira¹; Hiroyuki Wariishi²; Yoshinori Fujimura²; Daisuke Miura²; ¹Grad. Sch. Biores. Bioenviron. Sci., Kyushu Univ., Fukuoka, Japan; ²ICMRN, Kyushu Univ., Fukuoka, Japan; ³Fac. Arts and Sci., Kyushu Univ., Fukuoka, Japan
- WP 283 **Profiling of Regioisomeric Triacylglycerols in Edible Oils by Supercritical Fluid Chromatography/Tandem Mass Spectrometry;** Takeshi Bamba¹; Jae Won Lee¹; Toshiharu Nagai²; Naohiro Gotoh³; Eiichiro Fukusaki¹; ¹Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, Japan; ²Tsukishima Foods Industry Co., Ltd, Tokyo, Japan; ³Dept. Food Sci. Tech., Tokyo University of Marine, Tokyo, Japan
- WP 284 **Influence of the Silica Gel Layer Thickness on the Quality of TLC / MALDI Mass Spectra of Lipids;** Egidijus Machtejevas¹; Michael Schulz¹; Katerina Matheis²; Juergen Schiller³; ¹Merck Millipore, Merck KGaA, Darmstadt, Germany; ²Merck KGaA, Department of Bioanalytical Chemistry, Darmstadt, Germany; ³University of Leipzig, Faculty of Medicine, Leipzig, Germany
- WP 285 **Chromatography Couples through On-Line Liquid-Liquid Extraction with Electrospray Mass Spectrometry (CLL-MS) and Its Application to Lipoprotein Analysis;** Albert Koulman; Michael Osei; Julian L. Griffin; *Medical Research Council, Cambridge, UK*
- WP 286 **Pitfalls in Long-Term and Large-Scale LC-MS-based Lipidomics Studies of Human Plasma;** Tomas Cajka¹; Brian DeFelice¹; Carlos Leon¹; William Wikoff¹; Stanley Hazen²; Oliver Fiehn¹; ¹UC Davis Genome Center, Davis, CA; ²Cleveland Clinic Lerner Research Institute, Cleveland, OH
- WP 287 **Higher Resolution LC-MS and MS-MS Analysis of Lipid Extracts using Benchtop Orbitrap-based Mass Spectrometers and LipidSearch Software;** David Peake¹; Junhua Wang¹; Yasuto Yokoi²; Yingying Huang¹; ¹Thermo Fisher Scientific, San Jose, CA; ²MKI, Tokyo, Japan

- WP 288 **Characterization of Lipopolysaccharide Modifications in Select Antibiotic-Resistant Gram-negative Bacteria using Surface Acoustic Wave Nebulization Mass Spectrometry**; Lisa M. Leung; David R. Goodlett; Robert K. Ernst; *University of Maryland, Baltimore, Maryland*
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- WP 293 **Sample Preparation in Coated 96 Deep Well Plates for Clinical and Forensic Applications**; Susanne Nussbaumer¹; Wolfgang Weinmann¹; Michal Svoboda²; Roland Geyer²; Stefan König¹; ¹*Institut für Rechtsmedizin, Universität Bern, Bern, Switzerland*; ²*Tecan Schweiz AG, Männedorf, Switzerland*
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- WP 320 **Mass Spectrometric Method for Rapid Dereplication of Natural Product Platensimycin and Its Congeners in Producer Extracts**; Kithsiri Herath¹; Stephen Previs¹; Thomas Roddy¹; Athula Attygalle²; Sheo Singh¹; ¹Merck & Co., Kenilworth, NJ; ²Stevens Institute of Technology, Hoboken, NJ
- WP 321 **Techniques for DESI-MS Imaging of Fungal Cultures to Explore Chemical Interactions *in situ***; Vincent Sica; Huzefa Raja; Tamam El-Elimat; Nicholas Oberlies; UNCG, Greensboro, NC
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- WP 329 **Improving Molecular Structural Determination of a Pantetheine Analogue by Combining the Results of Alkali Metal Adduction Assisted EID & CAD**; Samantha L. Benson¹; David P. A. Kilgour²; Juan Wei¹; Mark Barrow¹; Manuela Tosin¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, UK; ²University of Maryland, Baltimore, Baltimore, MD
- WP 330 **Investigation of an Unprecedented Natural Non-Enzymatic Reaction with Laser Ablation Electrospray Ionization (LAESI) Mass Spectrometry Technology**; Lin Du¹; Haddon Goodman²; Robert Cichewicz¹; ¹University of Oklahoma, Norman, OK; ²Protea Biosciences, Inc., Morgantown, WV
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- WP 338 **Flow Injection Mass Spectrometric Fingerprinting (FIMS) Analysis for Differentiation of Three Black Cohosh Species**; Pei Chen¹; Huihui Huang¹; Jianghao Sun¹; Joe-Ann McCoy²; James Harnly¹; ¹USDA-ARS, Beltsville, MD; ²3The NC Arboretum Germplasm Repository, Asheville, NC
- WP 339 **Characterizing Compositional Differences in Isolated Populations of Little-Devil Frog Using LC-MS and GC-MS Analysis of Alkaloids**; Gary Byrd¹; Lauren O'Connell²; Sunia Trauger¹; Luis Coloma³; ¹FAS Small Molecule MS Core Facility, Harvard Univ., Cambridge, MA; ²FAS Center for Systems Biology, Harvard University, Cambridge, MA; ³Centro Jambatu de Investigación y Con. de Anfibios, Quito, Ecuador

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- WP 342 **Speciation without Chromatography Using Hydride Generation for the Selective Determination of Inorganic Arsenic**; Ásta Pétursdóttir^{1,3}; Stanislav Musil^{1,2}; Nils Friedrich¹; Andrea Raab¹; Helga Gunnlaugsdóttir³; Eva Krupp¹; Jorg Feldmann¹; Jenny Nelson⁴; ¹TESLA-Trace Elemental Speciation Laboratory, Aberdeen, UK; ²Institute of Analytical Chemistry of the ASCR, Brno, Czech Republic; ³Matis, Environment and Genetics Department, Reykjavik, Iceland; ⁴Agilent, Berkley, CA
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- WP 345 **Digital Ion Trap Mass Spectrometry for Radiological Debris Analysis;** [Theresa Evans-Nguyen](#)¹; Di Wang²; Friso H.W. Van Amerom³; ¹*Draper Laboratory, Tampa, FL*; ²*Johns Hopkins School of Medicine, Baltimore, MD*; ³*Mini-Mass Consulting, Inc., St. Pete Beach, FL*
- WP 346 **Use of Azo Dyes as Matrices and Chelators for the Detection of Metal Chelation Complexes using Matrix-Assisted Time-Of-Flight Mass Spectrometry;** Christopher Shiea¹; Yi-Lun Chen²; Min Zong Huang²; [Yeou-Lih Huang](#)¹; ¹*Dept. of Medical Lab Sci. & Biotech., KMU, Kaohsiung, Taiwan*; ²*Dep. of Chemistry National Sun Yat-Sen University, Kaohsiung, Taiwan*
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- WP 348 **Quantitative Analysis of Pesticides in QuEChERS Extracts using APGC/MS/MS;** [Douglas Stevens](#)¹; Dominic P T Roberts²; Ramesh Rao²; ¹*Waters Corporation, Milford, MA*; ²*Waters Corporation, Wimslow, UK*
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- WP 357 **Screening for Known and Unknown Food Residues and Contaminants using Accurate Mass LC-MS/MS and Automatic data Processing;** [Andre Schreiber](#)¹; David Cox¹; Nick Zhu²; Cheng Yuan Cai²; ¹*AB SCIEX, Concord, Canada*; ²*AB SCIEX, Shanghai, China*
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- WP 360 **Development of Retention Time Locked Accurate Mass EI Mass Spectral Database and Workflow for Pesticide Residue Screening Using GC/Q-TOF;** Samanta Uclés Duque¹; Noelia Belmonte Valles¹; Milagros Mezcua Peral¹; Amadeo Fernández-Alba¹; Klaus Wilmers²; Peter Fuerst²; [Sofia Aronova](#)³; Kai Meng³; Hong Chen³; Jennifer Gushue³; Maithilee Samant³; ¹*University of Almeria, Almeria, Spain*; ²*Chemical and Veterinary Analytical Institute, Muenster, Germany*; ³*Agilent Technologies, Inc., Santa Clara, CA*
- WP 361 **High-Throughput Determination of 5 Neonicotinoids in Honey using Differential Ion Mobility and LDTD-MS/MS;** [Sylvain Letarte](#); Gregory Blachon; Alex Birsan; Pierre Picard; Serge Auger; *Phytronix Technologies Inc., Quebec, QC*
- WP 362 **Evaluation of Different HILIC and Normal-Phase Approaches for the Liquid Chromatography/Mass Spectrometry-based Determination of Challenging Highly Polar Pesticides;** [Juan F Garcia-Reyes](#)¹; Andrea Vass²; Patricia Pérez-Ortega¹; Mihaly Dernovics²; Antonio Molina-Díaz¹; ¹*University of Jaen, Jaen, Spain*; ²*Corvinus University of Budapest, Budapest, Hungary*
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- WP 372 **Comprehensive Mass Spectrometry-Based Structural Determination of Small Subunit Ribosomal RNA: Characterization of N⁴-acetylcytidine and Identification of the Responsible Enzyme;** Masato Taoka¹; Daisuke Ishikawa¹; Yuko Nobe¹; Hideaki Ishikawa²; Hiroshi Nakayama^{3,4}; Yoshio Yamauchi¹; Nobuhiro Takahashi^{2,4}; Toshiaki Isobe^{1,4}; ¹Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; ²Department of Applied Biological Science, Tokyo Un, Tokyo, Japan; ³RIKEN, Wako, Japan; ⁴CREST, JST, Tokyo, Japan
- WP 373 **Steps toward Understanding the Molecular Basis of Bladder Carcinogenesis. Validation of a nanoLC-ESI-MS/MS platform and Application to 4-aminobiphenyl Dosing Studies;** Joshua Klaene¹; Arup Bhattacharya²; Yueheng Zhang²; James Glick¹; Paul Vouros¹; ¹Northeastern University, Boston, MA; ²Roswell Park Cancer Institute, Buffalo, NY
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- WP 375 **Molecular Motion in Porous Substrates under Electrospray Ionization Conditions;** Bin Hu; Zhongping Yao; *Department of Applied Biology and Chemical Technol, The Hong Kong Polytechnic University, Hong Kong, P. R. China*
- WP 376 **A Comparative Study of Ionization Efficiency of Solvent Assisted Inlet Ionization (SAIL) versus Electrospray Ionization (ESI);** Madeline Fenner; Charles McEwen; *University of the Sciences, Philadelphia, PA*
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- WP 379 **Investigation of the Chemical Interactions of the Triad: Sample, Solvent and Surface and Their Effects in DESI-MS Imaging Analysis;** Elaine Cristina Cabral; Wagner Polcelli; Demian Ifa; *York University, Toronto, Canada*
- WP 380 **Characterization of Ion Transport in Desorption Electrospray Ionization using Time-of-Flight Secondary Ion Mass Spectrometry;** Shin Muramoto; Thomas Forbes; Matthew Staymates; Greg Gillen; *National Institute of Standards and Technology, Gaithersburg, MD*
- WP 381 **Development of Solid Probe Assisted Electrospray Ionization Mass Spectrometry;** Mridul Kanti Mandal¹; Kenzo Hiraoka²; ¹University of Notre Dame, Notre Dame, IN; ²University of Yamanashi, Kofu, Yamanashi, Japan
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- WP 383 **Controlled *in situ* Formation of Molecular Ions, or Protonated Molecules, under Atmospheric Pressure Helium Plasma Ionization Mass Spectrometry (HePI-MS);** Athula B. Attygalle; Rekha Gangam; Julius Pavlov Julius Pavlov; Freneil Jariwala; *Stevens Institute of Technology, Hoboken, NJ*
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- WP 385 **First-Principle Transport Modeling of Protonated Peptides and Water Clusters in Ion Funnel and Nozzle-Skimmer Interfaces;** Sergey Gimelshein¹; Natalia Gimelshein²; Taylor Lilly³; Rebecca Webb³; Eugene Moskovets⁴; ¹University of Southern California, Los Angeles, CA; ²Gimel Inc., Montrose, CA; ³University of Colorado Colorado Springs, Colorado Springs, CO; ⁴MassTech Inc., Columbia, MD
- WP 386 **A VAMAS Interlaboratory Study for Desorption Electrospray Ionisation (DESI) Intensity Repeatability and Constancy;** Elzbieta Gurdak; Felicia M. Green; Martin P. Seah; Paulina D. Rakowska; Tara La Roche Salter; Ian S. Gilmore; Josephine Bunch; *National Physical Laboratory, Teddington, UK*
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- WP 390 **Paper Spray Mass Spectrometry (PS-MS) for the Quantification of Small Molecules Drugs in Plasma;** John Takyi-Williams¹; Haiqing Gong¹; Yang Wang²; Wenying Jian²; Kai Tang¹; ¹Nanyang Technological University, Singapore, Singapore; ²Janssen, a division of Johnson & Johnson, Shanghai, China
- WP 391 **Forensic Application of Solvent Assisted Ionization Inlet Mass Spectrometry (SAIL-MS);** Lyla Hassan; *USciences, Philadelphia, PA*
- WP 392 **The Analysis of Omega-3 Fatty Acid Oxidation by DESI and ESI-MS;** Raymond West¹; Rachel Marvin¹; Dragan Isailovic¹; Kenneth Hensley²; ¹University of Toledo, Toledo, OH; ²University of Toledo Medical Center, Toledo, OH
- WP 393 **Applications of Desorption Corona Beam Ionization-Mass Spectrometry;** Yuki Hashi¹; Shin-ichi Kawano¹; Changkun Li¹; Qian Sun¹; Taohong Huang¹; Tomoomi Hoshi²; Wenjian Sun³; ¹Shimadzu (China) Co., Ltd., Shanghai, China; ²Shimadzu Corporation, Kyoto, Japan; ³Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China
- WP 394 **Rapid Detection and Quantification with Novel Sorbent-Coated Mesh Substrate Using DART Mass Spectrometry;** Douglas B. Henderson; Johnny K. Ho; Yvette R. Hudson; William A. Harris; Danielle N. Dickinson; *Northrop Grumman, Linthicum Heights, MD*

- WP 395 **Single-probe Ionization Device: Development and Application to the Detection of Sulfated Post-Translationally Modified Proteins;** Rachel Vowcicefski; Ning Pan; Zhibo Yang; *University of Oklahoma, Norman, OK*
- WP 396 **Quantitative Analysis of Phosphoric Acid Esters in Aqueous Samples by Stir Bar Sorptive Extraction Combined with Isotope Dilution DART-HRMS;** Maxime Bridoux; Françoise Leprince; Frédéric Progent; Xavier Machuron-Mandard; *CEA, DAM, DIF, Arpajon, France*
- WP 397 **Exploration of Ambient Ionization Methods for Identification and Characterization of Biomarkers for Melanoma;** Michael T. Costanzo¹; Candice Ulmer¹; Shekher Mohan²; Nikolaus Gravenstein³; Richard A. Yost¹; ¹*Dept. of Chemistry, University of Florida, Gainesville, FL;* ²*CTRND, College of Medicine, University of Florida, Gainesville, FL;* ³*Dept of Anesthesiology, University of Florida, Gainesville, FL*
- WP 398 **Characterizing High-Valent Iron Porphyrin C-H Hydroxylation Reactions by Reactive Transmission Mode Desorption Electrospray Ionization Mass Spectrometry;** Kevin Peters; Kevin Parker; Richard Perry; *University of Illinois, Champaign, Illinois*
- WP 399 **Lipidomic Classification of Human Mammary Cancer Cells According to Metastatic Potential and Oncogene Expression by Desorption Electrospray Ionization Mass Spectrometry;** Heather Robison; Troy Comi; Seung Ryu; Richard Perry; *University of Illinois at Urbana-Champaign, Champaign, IL*
- WP 400 **Comparison of Paper Spray -MS/MS and Current Techniques for Screening Drugs of Abuse in Urine;** Joseph H Kennedy¹; Justin Wiseman¹; Brian C. Laughlin¹; Greg Lyons¹; Nicholas E Manicke²; Dianne Rampersaud³; Howard Lee³; ¹*Prosolia, Inc., Indianapolis, IN;* ²*IUPUI, Indianapolis, IN;* ³*Clinitox Diagnostix, Mississauga, Ontario*
- WP 401 **Characterization of Ammonium Nitrate Vapor with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry;** G. Asher Newsome¹; E. Lucus Steinkamp²; Braden C. Giordano³; ¹*Nova Research, Alexandria, VA;* ²*National Research Council, Washington, DC;* ³*U.S. Naval Research Laboratory, Washington, DC*
- WP 402 **Applications of Confined DART (Direct Analysis in Real Time) Ion Source for Online *in vivo* Analysis of Human Breath;** Yue Li; *The University of Maryland, College Park, MD*
- WP 403 **Effective Use of Direct Ionization Mass Spectrometry for Screening Food, Packaging & Cosmetics;** Luke Ackerman¹; Karim Bentayeb²; Timothy Begley¹; ¹*FDA Center for Food Safety, College Park, MD;* ²*Analytical Chem., Univ. Zaragoza, Zaragoza, Spain*
- WP 404 **Rapid Determination of Clenbuterol in Pig's Urine by Direct Analysis in Real Time Tandem Mass Spectrometry;** Zong Yang¹; Xiaokun Duan¹; Charles C. Liu¹; Qinghe Zhang²; Xiuqin Li²; Dazhou Chen²; ¹*ASPEC Technologies Limited, Beijing, China;* ²*National Institute of Metrology, Beijing, China*
- WP 405 **Mass Spectrometry Imaging of Skin Wound Healing Biomarkers Using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS);** Pamela Cantrell¹; Callee Walsh¹; Greg Kilby¹; Tanya Shaw²; ¹*Protea Biosciences Group, Inc., Morgantown, WV;* ²*St. George's, University of London, London, UK*
- WP 406 **Fingerprint of Anthocyanins from Two Varieties of Beans using ESI-MS and Direct Infusion;** Carlos Fidelis¹; Renata Sancho²; Marcos N Eberlin¹; Glauca Pastore²; ¹*Institute of Chemistry - University of Campinas, Campinas, Brazil;* ²*Faculty of Food Eng. University of Campinas, Campinas, Brazil*
- WP 407 **Rapid Determination and Semi-Quantitative Analysis of Dicyandiamide in Milk by Direct Analysis in Real Time (DART) Time-Of-Flight Mass Spectrometry;** Liya Zhang¹; Wei Yong²; Xiaogang Chu²; Tianyang Guo¹; Yiyang Dong¹; Xiaokun Duan³; Zong Yang³; Charles C. Liu³; ¹*Beijing University of Chemical Technology, Beijing, China;* ²*Chinese Academy of Inspection and Quarantine, Beijing, China;* ³*ASPEC Technologies Limited, Beijing, China*
- WP 408 **Rapid Screening of the SAMHSA (NIDA) Panel in Urine using DSA/TOF;** Avinash Dalmia¹; Leslie Sullivan¹; George Perkins¹; Craig M. Whitehouse²; ¹*PerkinElmer, Shelton, CT;* ²*PerkinElmer, Branford, CT*
- WP 409 ***In situ* Detection of Pnictogen Elements in Minerals by Ambient-Pressure Helium Plasma Ionization Mass Spectrometry;** Julius Pavlov; Athula Attygalle; *Stevens Institute of Tech, Hoboken, NJ*
- WP 410 **Detection and Quantification of Naturally Occurring Ions in Ethylene Flames and the Effect of Ethanol Addition on Polyaromatic Hydrocarbon Formation;** Thomas Bierkandt¹; Denis A. Knyazkov²; Erdal Akyildiz¹; Tina Kasper¹; ¹*University of Duisburg-Essen, Duisburg, Germany;* ²*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*
- WP 411 **Quantitative Assessment of Amino Acid Profiles in Foodstuffs with Microwave Hydrolysis and Desorption Electrospray Ionization Mass Spectrometry;** Jonathan Person; Christopher Mulligan; *Illinois State University, Normal, IL*
- WP 412 **Molecular Ionization from Carbon Nanotube Paper;** Rahul Narayanan¹; Depanjan Sarkar¹; R. Graham Cooks²; Pradeep T. ¹*IIT Madras, Chennai, India;* ²*Purdue University, West Lafayette, IN*
- WP 413 **A Novel Approach to Determine Tyrosine, 3-Chlorotyrosine and 3-Nitrotyrosine in Human Plasma by DART-MS/MS;** Yu-Qiao Song¹; Jie Liao¹; Cheng Zha¹; Bin Wang¹; Zong Yang²; Charles C. Liu²; ¹*Medical Exp & Anal Ctr PLA General Hospital, Beijing, China;* ²*ASPEC Technologies Limited, Beijing, China*
- WP 414 **A Rapid Procedure Using Direct Analysis in Real Time-Mass Spectrometry to Screen for Adulterants in Herbal Dietary Supplements;** Xiaokun Duan¹; Yu Zhao²; Lihui Yin²; Changqin Hu²; Zong Yang¹; Charles C. Liu¹; ¹*ASPEC Technologies Limited, Beijing, China;* ²*National Institutes for Food and Drug Control, Beijing, China*
- WP 415 **Rapid Quantification of Drugs in Blood Using Solid Phase Microextraction Coupled to Thermal Desorption Electrospray Ionization Mass Spectrometry;** Chin-Hsiung Wang¹; Min Zong Huang²; Jo-Han Chou²; Jentaie Shiea²; ¹*Protech Pharmaservices Co., Taipei, Taiwan;* ²*National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- WP 416 **Authenticity Assessment of Imported Olive Oil using Direct Analysis in Real Time Mass Spectrometry;** Fengqi Wu¹; Zhenfeng Yue¹; Xiaokun Duan²; Zong Yang²; Honghui Hua¹; Weidong Wu¹; Charles C. Liu²; ¹*Entry-Exit Inspection and Quarantine Bureau, Shenzhen, China;* ²*ASPEC Technologies Limited, Beijing, China*
- WP 418 **Atmospheric Pressure Photoionization: Establishing the Ionization Limits for Synthetic Organic and Organometallic Complexes;** Konstantin O. Zhurov; Laure Menin; Yury O. Tsybin; *Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*
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- WP 421 **Targeted Exposomics: Profiling Urinary Organic Acids;** Anthony Macherone^{1,2}; Timothy Conjelko¹; ¹*Agilent Technologies, Wilmington, DE;* ²*Johns Hopkins University, Baltimore, MD*

- WP 422 **Using Fine Needle Aspiration Combined with Matrix-Assisted Laser Desorption Ionization/Time-of-Flight Mass Spectrometry to Diagnose Breast Cancer;** Hung Su¹; Ya-Fei Bao¹; Yi-Tzu Cho²; Jentaie Shiea¹; Pei-Yung Nien³; Ya-Hui Chang³; Ming-Feng Hou³; ¹National Sun Yat-Sen Univ., Kaohsiung, Taiwan; ²Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan; ³Cancer Research Center, Kaohsiung Medical Univ., Kaohsiung, Taiwan
- WP 423 **A Validated LC-MS/MS Method for Rapid Methotrexate Determination in Human Saliva and Its Application to an Excretion Evaluation Study;** Igor Rodin; Arkady Braun; Andrey Stavrianidi; Irina Ananieva; Oleg Shpigun; *MSU, Moscow, RU*
- WP 424 **Detecting Lymph Node Metastases *in-vivo* with Rapid Evaporative Ionization Mass Spectrometry;** Julia Balog^{1,2}; Attila Enyedi³; Orsolya Nagyhazi³; Laszlo Toth³; Peter Varga²; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Medimass Ltd, Budapest, Hungary; ³Debrecen University, Debrecen, Hungary
- WP 425 **Using MRM³ for Removing Interferences in Plasma Metanephrines Analysis: The Quest for an Improved Clinical Service;** Michael Wright¹; Rebecca Thomas¹; Chris Hodgkins²; ¹SEALS, Prince of Wales Health Pathology, Sydney, Australia; ²ABSciex, Sydney, Australia
- WP 426 **A HILIC-ESI-MS/MS Method for the Quantification of Free and Total Carnitine for Patient Care;** Tiffany Thomas; Jorge Sepulveda; Michael Pesce; *Columbia University Medical Center, New York, NY*
- WP 427 **An Improved Internal Standard Ratio Quantitation Technique for Clinical Diagnostics;** Brian Rappold; *Essential Testing, Collinsville, IL*
- WP 428 **Burden of Proof: Providing Clinical Confidence in the Face of Analytical Fallacies;** Martin Green; Christopher Shuford; Patricia Holland; Russell Grant; *Laboratory Corporation of America, Burlington, nc*
- WP 429 **Measurement of Low Level Endogenous Biomarkers for Use in Clinical Diagnostics;** Stacy Dee; Christopher Shuford; Matthew Crawford; Patricia Holland; Yvonne Wright; Martin Green; Russell Grant; *LabCorp, Burlington, NC*
- WP 430 **A Novel Approach for the Diagnosis of Gaucher Disease using Flow Injection Tandem Mass Spectrometry;** Jie Chen¹; Michael Bennett^{1,2}; ¹Children's Hospital of Philadelphia, Philadelphia, PA; ²University of Pennsylvania, Philadelphia, PA
- WP 431 **An LC-ESI-MS/MS Method for Plasma Oxysterols Derivatized as Dimethylaminobutyrate Esters;** David W. Johnson¹; Sara Boenzi²; ¹SA Pathology/Women's and Children's Hospital, North Adelaide, Australia; ²Ospedale Pediatrico Bambino Gesù, Rome, Italy
- WP 432 **Simultaneous Measurement of 6 α -Hydroxy-Melatonin Sulfate and Cortisol in Human Urine by LC/MS/MS;** Bhasin Shalender; Xiaohong Chen; Gordon Harold Williams; Liming Peng; *Brigham and Women's Hospital, Boston, Massachusetts*
- WP 433 **A Fast and Effective Approach for the Analysis of Urinary Cortisol, Cortisone, Prednisolone and Prednisone using SPE and LC-MS/MS;** Xianrong (Jenny) Wei; Sean Orłowicz; *Torrance, ca*
- WP 434 **Development of a Sensitive Ultrapressure Liquid Chromatography Tandem Mass Spectrometry Method for Quantification of Dihydrotestosterone in Human Serum;** Karina Helena Morais Cardozo; Jessica Silva Salgueiro; Valdemir Melechco Carvalho; *Fleury Group, São Paulo, Brazil*
- WP 435 **Enhanced Application Stability utilizing SPLC-MS/MS;** Christopher L. Esposito¹; Francois A. Espourteille²; ¹Thermo Scientific, Franklin, MA; ²Thermo Fisher Scientific, Franklin, MA
- WP 436 **Quantitation of Reduced and Oxidized Glutathione and Cysteine in Acid-Preserved Samples by Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry;** Alan W. Taylor; Deborah Hobbs; Debbie J. Mustacich; Balz Frei; *Oregon State University, Corvallis, OR*
- WP 437 **Ultrafast Antiretroviral Drug Analysis in Human Serum;** Kari Schlicht; Vaughn Miller; William A. Lamarr; *Agilent Technologies, Wakefield, MA*
- WP 438 **Plasma Citric Acid Cycle Intermediates Levels by LC-MS/MS - A Prospective Application in Diagnosis of Mitochondrial Disorders;** Yana Sandler^{1,2}; Richard Kelley^{1,2}; ¹Kennedy Krieger Institute, Division of Metabolism, Baltimore, MD; ²Johns Hopkins University, Department of Pediatrics, Baltimore, MD
- WP 439 **Direct Measurement of Pancreatic Polypeptide in Human Serum and plasma by Immuncapture-Liquid-Chromatography-Tandem Mass Spectrometry;** Hernando Escobar; Mark M. Kushnir; Alan L. Rockwood; A. Wayne Meikle; *ARUP Laboratories-University of Utah, Salt Lake City, UT*
- WP 440 **Fast and Robust LC-MS/MS Method for Determination of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood using Automated Extraction;** Anders Blomgren; *Clinical Chemistry, Lund, Sweden*
- WP 441 **UPLC-MS/MS Multiplex Analysis for Mass or High-Risk Screening of Creatine Synthesis and Transport Disorders, Triple H Syndrome and OTC Deficiency;** Pamela Lavoie; Bruno Maranda; Christiane Auray-Blais; *Université de Sherbrooke/CRC-CHUS, Sherbrooke, Canada*
- WP 442 **Mass Spectrometry-Based Elemental Bioimaging and Speciation Analysis as Diagnostic Tools for Nephrogenic Systemic Fibrosis;** Uwe Karst; Kristina Wentker; Marvin Birka; Christoph Wehe; Michael Holtkamp; Michael Sperling; *University of Münster, Münster, Germany*
- WP 443 **Multiplex Newborn Screening of Lysosomal Storage Disorders using Flow Injection Tandem Mass Spectrometry;** Mariana Barcenás¹; Martin Sadilek¹; C. Ronald Scott³; Frantisek Turecek¹; Michael Gelb^{1,2}; ¹University of Washington, Department of Chemistry, Seattle, WA; ²University of Washington, Dept. of Biochemistry, Seattle, WA; ³University of Washington, Dept. of Pediatrics, Seattle, WA
- WP 444 **Clinical Screening of Hemoglobinopathies using Top Down Mass Spectrometry;** James Scrivens¹; Smith Julia³; Sarah Nicolle⁴; Jane Newbold⁴; Krisztina Radi²; ¹Univ of Warwick, Coventry, UK; ²University of Warwick - Life Sciences, Coventry, UK; ³Bruker, Coventry, UK; ⁴Coventry and Warwickshire Hospital, Coventry, UK
- WP 445 **Top-down MS/MS Hemoglobinopathy Screening of Neonatal Samples;** Roger Theberge¹; Carolyn Hoppe²; Christian Heckendorf¹; David H. K. Chui¹; Catherine E. Costello¹; Mark E. McComb¹; ¹Boston University School of Medicine, Boston, MA; ²Children's Hospital & Research Center Oakland, Oakland, CA
- WP 446 **Towards the Development of Saliva-Based Malaria Diagnostics: Mass Spectrometry Based Identification of Gametocyte Proteins in Human Saliva;** Dingyin Tao¹; Isabelle Morlais²; Tamaki Kobayashi¹; William John Moss¹; Rhoel R Dinglasan¹; ¹Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; ²Laboratoire de Recherche sur le Paludisme, Yaoundé, Cameroun

- WP 447 **Apolipoprotein E ϵ 2, ϵ 3 and ϵ 4 Isoform Specific Quantification in Human Sera using LC-MRM;** Christophe Hirtz¹; Jérôme Vialaret¹; Susanna Schraen²; Benlian Pascale³; Sandrine Mary³; Laurent Tiers¹; Baptiste Gor¹; Pauline Bros¹; Constance Delaby¹; Audrey Gabelle^{1,4}; Sylvain Lehmann¹; ¹CHU de Montpellier and UM1, Montpellier, France; ²Inserm U837, Lille, France; ³U4M, Lille, France; ⁴Centre Mémoire Ressources Recherche LR, Montpellier, France
- WP 448 **Sample Treatment and Stability of Urine Samples from Patients with APRT Deficiency Used in Mass Spectrometry Based Clinical Diagnostics;** Margret Thorsteinsdottir^{1,2}; Finnur F Eiriksson^{1,2}; Hrafnhildur L Runolfsdottir¹; Vidar O Edvardsson³; Runolfur Palsson^{1,3}; ¹University of Iceland, Reykjavik, Iceland; ²ArcticMass, Reykjavik, Iceland; ³Landspítali – The National University Hospital, Reykjavik, Iceland
- WP 449 **Development and Validation of 2D-LC/MS/MS Method for Quantitative Analysis of 1 α ,25-Dihydroxyvitamin D3 in Human Serum;** Daryl Kim Hor Hee¹; Lawrence Soon-U Lee¹; Edwin Zhi Wei Ting²; Jie Xing²; Sandhya Nargund²; Miho Kawashima³; Zhaoqi Zhan²; ¹Department of Medicine Research Laboratories, National University of Singapore, 6 Science Drive, 2, Singapore 117546; ²Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, 79 Science Park Drive, #02-01/08, Singapore 118264; ³Global Application Development Centre, Shimadzu, Corporation, 1-3 Kanda Nishihiki-cho, Chiyoda-ku., Tokyo 101-8448, Japan
- WP 450 **The Analysis of Vitamin D Metabolites in Serum by LC-MS/MS;** Shun-Hsin Liang; Sharon Lupo; Restek, Bellefonte, PA
- WP 451 **Stability of 25-Hydroxyvitamin D Metabolites in Calibration Solutions used for LC-MS Assays;** Mary Bedner; Katrice Lipka; NIST, Gaithersburg, MD
- WP 452 **Systematic Investigation of Isobaric Interferences in Vitamin D Analysis by Differential Ion Mobility Spectrometry and FTICR Mass Spectrometry;** Florian Meier¹; Timon Geib¹; Pascal Schorr¹; Yulin Qi¹; Mark Bokhart²; Elias Rosen²; David Muddiman²; Dietrich Volmer¹; ¹Saarland University, Saarbrücken, Germany; ²North Carolina State University, Raleigh, NC
- WP 453 **Value Assignment of Vitamin D Metabolites in Vitamin D Standardization Program (VDSP) Serum Samples;** Karen Phinney¹; Johanna Camara²; Susan Tai²; Linda Thienpont³; Blaza Toman²; Antonio Possolo²; Christopher Sempos⁴; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²NIST, Gaithersburg, MD; ³Ghent University, Ghent, Belgium; ⁴NIH Office of Dietary Supplements, Bethesda, MD
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- WP 454 **Shotgun Proteomics of Human Sputum Identifies Potential Cancer and Metabolic Biomarkers from Exposures to Diesel and Biodiesel Exhaust;** Aaron Mehus^{1,2}; Sally Littau²; Eric Lutz²; Jeffrey Burgess²; ¹University of Arizona College of Medicine, Tucson, AZ; ²University of Arizona College of Public Health, Tucson, AZ
- WP 455 **Deconvolution of Chemical Signals from Endangered African Wild Dogs;** Peter Apps¹; John Moncur²; ¹Botswana Predator Conservation Trust, Maun, Botswana; ²SpectralWorks Ltd, Runcorn, UK
- WP 456 **An LC/MS/MS Screening Approach to Discover Unknown Hemoglobin Adducts;** Henrik Carlsson; Hans von Stedingk; Ulrika Nilsson; Margareta Törnqvist; Stockholm University, Stockholm, Sweden
- WP 457 **Proteomic Investigation of Sera and Saliva Samples from Children with Autism Spectrum Disorder (ASD) and Matched Controls;** Kelly Wormwood¹; Armand G. Ngounou Wetie¹; Izabela Sokolowska¹; Katherine Beglinger¹; Jeanne Ryan²; Alisa Woods¹; Costel Darie¹; ¹Clarkson University, Potsdam, NY; ²SUNY Plattsburgh, Plattsburgh, NY
- WP 458 **Mass Selected Site-Specific Core-Fucosylation of Ceruloplasmin in Alcohol-Related Hepatocellular Carcinoma;** Haidi Yin¹; Zhenxin Lin¹; Song Nie¹; Jing Wu¹; Zhijing Tan¹; Jianhui Zhu¹; Jianliang Dai²; Ziding Feng²; Jorge Marrero³; David Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Texas MD Anderson Cancer Center, Houston, TX; ³University of Texas Southwestern Medical Center, Dallas, TX
- WP 459 **Mass Spectrometric Investigation of Potential Biomarkers of Cold Stress in Saliva;** Rachel Marvin; Brooke Saepoo; Jonathan Tomko; Dr. Kenneth Hensley; Dr. David Giovannucci; Dr. Dragan Isailovic; University of Toledo, Toledo, Ohio
- WP 460 **Discovery-to-Targeted Biomarkers and Therapeutic Targeted Pipeline;** Rebeca Kawahara¹; Gabriela Meirelles¹; Henry Herbele²; Daniela Granato¹; Sami Yokoo¹; Rafael Canevarolo⁴; Romênia Domingues¹; Flavia Winck¹; Ana Carolina Prado⁸; Paulo Filgueiras⁵; Karen Cruz⁹; Alexandre Barbuto⁹; Ronei Poppi⁵; Rosane Minghim²; Guilherme Telles⁷; Felipe Paiva³; Jay Fox⁶; Alan Santos-Silva³; Ricardo Coletta³; Nicholas Sherman⁶; Adriana Paes Leme¹; ¹Laboratório Nacional de Biociências, Campinas, Brazil; ²Instituto de Ciências Matemáticas e de Computação, São Carlos, SP; ³Faculdade de Odontologia de Piracicaba, UNICAMP, Piracicaba, SP; ⁴Centro Infantil Boldrini, Campinas, SP; ⁵Instituto de Química, UNICAMP, Campinas, SP; ⁶W. M. Keck Biomedical Mass Spectrometry Lab, Charlottesville, VA; ⁷Instituto de Computação, UNICAMP, Campinas, SP; ⁸Instituto do Câncer do Estado de São Paulo, São Paulo, SP; ⁹Instituto de Ciências Biomédicas, USP, São Paulo, SP
- WP 461 **Use of Mass Spectrometry for Identification of Biomarkers of Exposure to Flame Retardants;** Manori Silva¹; Donald Hilton¹; Jonathan Furr²; L Earl Gray²; James Preau¹; Antonia Calafat¹; Xiaoyun Ye¹; ¹CDC, Atlanta, GA; ²FDA, Research Triangle Park, NC
- WP 462 **Mass Spectrometry in Clinical Diagnosis: A Preliminary Application in Tumor Cellular Proteomics for Biomarker Discovery;** Ming-Hui Yang¹; Yung-Yu Chang²; Tsung-Min Wang²; Yu-Chang Tyan²; ¹National Applied Research Laboratories, Hsinchu, Taiwan; ²Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 463 **Comparative Label-Free Proteomics of Pericytes, Circulatory Fibrocytes, in contact with Vascular Endothelium (huVEC);** Harsha P. Gunawardena²; Jingjing Li¹; ¹Department of Surgery, School of Medicine, UNC-Chapel Hill, NC; ²Program in Molecular Biology & Biotechnology, UNC-Chapel Hill, NC
- WP 464 **Lipids Regulators in B-cell Chronic Lymphocytic Leukemia;** Huan Kang; David Bearss; John Prince; Brigham Young University, Provo, Utah
- WP 465 **Identification of New Toxicity Biomarkers for Microbicides;** Benben Song¹; Scott Fields²; Bazeza Rasoul¹; Carsten Alt²; Mary J. Tanga²; Jon Mirsalis²; Annalisa D'Andrea²; ¹SRI International, Harrisonburg, VA; ²SRI International, Menlo Park, CA
- WP 466 **Correction of Precursor and Product Ion Abundances in Order to Standardize CID Spectra and Improve Ecom50 Accuracy for Non-Targeted Metabolomics;** Ritvik Dubey¹; David Grant¹; Dennis Hill¹; Steven Lai²; Chen

- Ming Hui³; ¹University of Connecticut School of Pharmacy, Storrs, CT; ²Waters Corporation, Boston, MA; ³University of Connecticut, Dept. of Statistics, Storrs, CT
- WP 467 **Proteome Analysis of Extracellular Vesicles from Patients with Systemic Sclerosis; Ole Østergaard¹**; Line V. Iversen²; Søren Jacobsen³; Niels HH Heegaard¹; ¹Statens Serum Institut, Copenhagen, Denmark; ²Department of Dermatology, Bispebjerg Hospital, Copenhagen, Denmark; ³Department of Rheumatology, Rigshospitalet, Copenhagen, Denmark
- WP 468 **Proteomic and Informatic Approaches in the U-BIOPRED Severe Asthma Project: Large-Scale MS^E, Data Mining, Machine Learning, and Topological Data Analysis; Dominic Burg^{1,2}**; Doroteya Staykova¹; Xian Yang³; Yike Guo³; Ratko Djukanović²; Paul Skipp¹; U-BIOPRED Consortium^{4,5}; ¹Centre for Proteomic Research, Uni of Southampton, Southampton, UK; ²NIHR Respiratory Biomedical Research Unit, Southampton General Hospital, UK; ³Imperial College, London, UK; ⁴European Lung Foundation, Sheffield, UK; ⁵Innovative Medicines Initiative, Bruxelles, Belgium
- WP 469 **A Quantitative Proteomic Approach to Study the Interplay between Colorectal Cancer and the Immune System; Evelynne Maes^{1,2}**; Geert Baggerman^{2,3}; Dirk Valkenborg^{2,3}; Bart Landuyt¹; Liliame Schoofs¹; Hans Prenen⁴; Inge Mertens^{2,3}; ¹KU Leuven, Functional Genomics and Proteomics lab, Leuven, Belgium; ²Flemish Institute for Technological Research (VITO), Mol, Belgium; ³Center for Proteomics, Antwerp, Belgium; ⁴Digestive oncology unit, UZ Leuven, Leuven, Belgium
- WP 470 **Proteomic Analysis of Doxorubicin-induced Cardiotoxicity in Mice; Zhijun Cao**; Yuan Gao; Varsha G. Desai; James C. Fuscoe; Li-Rong Yu; *National Center for Toxicological Research, FDA, Jefferson, AR*
- WP 471 **Targeted and Untargeted Mass Spectrometry for Identification of Metabolomic Changes in a Human Epigenetic Model of Chronic Stress; Constance Sobsey¹**; Jun Han¹; Clemens Kirschaum²; Karl Radtke³; Thomas Elbert³; Christoph Borchers^{1,4}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²Dresden University of Technology, Psychology Dept, Dresden, Germany; ³Universität Konstanz, Clinical Psychol. & Neurol., Konstanz, Germany; ⁴UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 472 **Mass Spectrometric Identification of Lipids Associated with Pulmonary Aspergillus Infections; Rita Semis**; Gabriel B. Gugiu; Teresa B. Hong; Markus Kalkum; *City of Hope, Duarte, CA*
- WP 473 **High Sensitivity Enrichment of Glycopeptides from Complex Biological Samples using Metal Organic Frameworks; Hongqiang Qin¹**; Chunli Fang¹; Zhichao Xiong¹; Guang Huang¹; Junfeng Huang¹; Xiuping Yan²; Shun Feng¹; Mingliang Ye¹; Hanfa Zou¹; ¹Key Laboratory of Separation Science for Analytica, Dalian, China; ²Nankai University, Tianjin, China
- WP 474 **Proteome and Glycoproteome Analyses for Breast Cancer Biomarker Discovery with Nipple Discharge Using Two-Dimensional Nano LC/Nano-ESI-MS; Sadamu Kurono^{1,2}**; Norifumi Kobayashi^{1,2}; Tomoyuki Nakajima³; Shuji Matsuura¹; Nariaki Matsuura¹; Haruki Oishi¹; ¹Osaka University Graduate School of Medicine, Suita, Osaka, Japan; ²Wako Pure Chemical Industries, Ltd., Osaka, Osaka, Japan; ³Shinshu University Hospital, Matsumoto, Nagano, Japan
- WP 475 **Laser Capture Microdissection for Advanced LC-MS Discovery of Specific Cell Populations within Tissue Samples; Lisa Staunton¹**; Marie Reidy²; Rosina Lis³; Kieran Wynne¹; Belinda Hernandez¹; Steve Finn²; William Watson¹; Massimo Loda³; Michaela Bowden³; Stephen Pennington¹; ¹Conway Institute, Dublin 4, Ireland; ²St. James' Hospital, Dublin, Ireland; ³Dana Faber Cancer Institute, Boston, MA
- WP 476 **Identification of New Quorum Sensing Molecules in Complex Media using High resolution Mass Spectrometry and MS-MS Fragmentation; Daniel Todd¹**; David Zich¹; Keivan Etefagh¹; Alexander Horswill²; Nadja Cech¹; ¹Univ. of N. Carolina Greensboro, Greensboro, NC; ²University of Iowa, Iowa City, IA
- WP 477 **Profiling of Proteins and Polar Metabolites in Rat Tears by High Resolution Mass Spectrometry; Toshiyuki Mikami**; Takafumi Matsumoto; Tsuyoshi Noguchi; *Dainippon Sumitomo Pharma, Osaka, Japan*
- WP 478 **Human Eye Peptidomics for More Efficient Screening of Donor Corneal Tissue; Bharath Kumar Raghuraman¹**; Martijn Pinkse¹; Mervin Pieterse¹; Valerie Bentivegna¹; Marieke Bruinsma²; Hans Frank²; Gerrit Melles²; Peter D. Verhaert¹; ¹Delft University of Technology, Delft, Netherlands; ²NIIOS, Rotterdam, Netherlands
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- WP 479 **Ultra-Sensitive Stable Isotope Dilution Liquid Chromatography-Tandem Mass Spectrometry Method for Quantification of Estrogens and Estrogen Metabolites in Human Serum; Qingqing Wang^{1,2}**; Clementina Mesaros¹; Lisa Bottalico¹; Kannan Rangiah³; Ian A. Blair¹; ¹University of Pennsylvania, Philadelphia, PA; ²Beijing Institute of Radiation Medicine, Beijing, China; ³Center for Cellular and Molecular Platforms, Bangalore, India
- WP 480 **Development and Validation of LC-MS/MS Methods for Quantitative Determination of Key Kynurenine Pathway Metabolites in Human Plasma and Cerebrospinal Fluid; Mike Allen¹**; Ben Begley¹; Kelvin Chan²; David Delinsky¹; Roger Demers³; Valerie Kempf¹; Kathryn Lyons⁴; Brian Nofsinger¹; Kendall Powell¹; Daren Stephens¹; Weslyn Ward¹; Daria Wentzel³; Patricia Wheelan¹; Ignacio Munoz²; Ladislav Mrzljak²; Leticia Toledo-Sherman²; Celia Dominguez²; ¹Tandem Labs, Durham, NC; ²CHDI Foundation, Princeton, NJ; ³Tandem Labs, West Trenton, NJ; ⁴PK Consultant, Holland, NY
- WP 481 **Profiling EGFR Kinase Inhibitor Resistance Pathways in Non-Small Lung Cancer Cells; Ryan Bomgardner¹**; Gregory Botting²; Ryan Jacobs²; Rosa Viner³; Neelu Puri²; John C. Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL; ²University of Illinois at Chicago, Rockford, IL; ³ThermoFisher Scientific, San Jose, CA
- WP 482 **Determining the Functional Role of Keratin Filament in Apoptosis via the PI3K/Akt Signaling Pathway using LTQ Orbitrap MS/MS Analysis; Nancy Fernandes**; Nicole Morin Jaskiewicz; Feixia Chu; Dave Townson; *University of New Hampshire, Durham, NH*
- WP 483 **Development and Qualification of a Method for Quantitative Determination of Multiple Bile Acids with microLC/MS/MS; Michael Johnson**; *Takeda Pharmaceuticals, Cambridge, MA*
- WP 484 **Quantitative Analysis of the Biomarkers Dopamine, DOPAC (3,4-Dihydroxyphenylacetic Acid), and HVA (Homovanillic Acid) in Rat Brain Tissue Homogenate; Angela Qi Shen**; Wenlin Yuan; Ritika Kurian; Steven Wiltshire; *Agilux Laboratories, Worcester, MA*
- WP 485 **Measuring the Cooked Meat Carcinogen 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in Dyed Hair; Jingshu Guo¹**; Kim Yonemori²; Kami K. White²; Lynne R. Wilkens²; Loic Le Marchand²; Robert Turesky¹; ¹University of Minnesota, Minneapolis, MN; ²University of Hawaii, Honolulu, HI

- WP 486 **γ -Aminobutyric Acid and Glutamic Acid as Biomarkers of Neuropathic Pain Caused by Palictaxel;** Pei Li; Benjamin Albrecht; Hanrong Weng; Michael Bartlett; *University of Georgia, Athens, GA*
- WP 487 **Analyte Stability, Selectivity, and Importance of Sample Preparation for the Accurate Determination of LPA, a Potential Stratification Biomarker, in Biofluids;** Joelle Onorato; Petia Shipkova; Anne Minnich; Anne Aubry; John Easter; Adrienne Tymiak; *Bristol-Myers Squibb, Princeton, NJ*
- WP 488 **A Novel LC-MS/MS Method for Quantitation of Three Free Form Fatty Acids in Human Plasma;** Dawei Zhou¹; Du-Shieng Chien²; Xiping Fang¹; Xingye Yang¹; Jinn Wu¹; ¹*XenoBiotic Laboratories, Inc., Plainsboro, NJ*; ²*Efficient Pharma Management Corporation, Taipei, Taiwan*
- WP 489 **Membrane Protein Enrichment Strategy to Identify Biomarker Candidates in Alzheimer's Disease using Quantitative Mass Spectrometry;** Sravani Musunuri; Kim Kultima; Martin Ingelsson; Lars Lannfelt; Jonas Bergquist; Ganna Shevchenko; *Uppsala University, Uppsala, Sweden*
- WP 490 **Biomonitoring of Methylene Diphenyl Diisocyanate Adducted to Lysine Amino Acids (K-MDA) in Rat Urine;** Leah Luna; Michael Bartels; Dan Markham; Kathy Brzak; *The Dow Chemical Company, Midland, MI*
- WP 491 **Multiple Biomarker Analysis of Breast Cancer Clinical Biopsies using MRM MS;** Chris Sutton¹; Sadr-ul Shaheed¹; Andreas Hadjisavvas²; Kyriacos Kyriacou²; Paul Loadman¹; ¹*Institute of Cancer Therapeutics, Bradford, UK*; ²*Cyprus Institute of Neurology and Genetics, Nicosia, Cyprus*
- WP 492 **Nanoprobe-Based Affinity Multiple Reaction Monitoring (MRM) Approach for Verification of Hepatocellular Carcinoma (HCC) Biomarkers;** Mira Anne C. Dela Rosa^{1,2}; Kai-Yi Wang^{1,2}; Rofeamor P. Obena³; Rey Y. Capangpangan^{2,3}; Pei-Yi Lin³; Yu-Ju Chen³; ¹*Department of Chemistry, National Taiwan University, Taipei, Taiwan*; ²*Taiwan International Graduate Program, Taipei, Taiwan*; ³*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*
- WP 493 **A Strategy for MRM-based Verification of Bladder Cancer Protein Biomarkers;** Cheng-Han Tsai¹; Ting Chung¹; Chien-Lun Chen²; Jau-Song Yu¹; Yi-Ting Chen¹; ¹*Chang Gung University, Tao-Yuan, Taiwan*; ²*Chang Gung Memorial Hospital, Tao-Yuan, Taiwan*
- WP 494 **Development of MRM Methods for Clinical Analysis of Urinary Myoglobin;** James Hribar¹; Jon Klein^{1,2}; Daniel Wilkey¹; Kenneth McLeish^{1,2}; Michael Merchant¹; ¹*Department of Medicine-Nephrology, Louisville, KY*; ²*Veterans Administration Medical Center, Louisville, KY*
- WP 495 **SRM-based Kinetic Measurements of Biomarkers for Cardiovascular Disease, Utilizing Isotope Enrichment Studies in Non-Human Primates and Human Subjects;** Fang Xie; Brooke Rock; Maurice Emery; Dan Rock; *Amgen, Seattle, WA*
- WP 496 **Method Development for the Quantitation of a Urine Biomarker for Acute Kidney Injury using a QTRAP® Mass Spectrometer;** Dietrich Merkel; Christian Baumann; Jörg Dojahn; *AB SCIEX, Darmstadt, Germany*
- WP 497 **An Integrated High-Throughput Protein Quantification Workflow by Robotic Sample Preparation and Selected Reaction Monitoring in Large-Scale Biomarker Study;** Xiaoqian Liu^{1,2}; Qin Fu^{1,2}; Michael P Kowalski³; Graham J Threadgill⁴; Christie Hunter⁵; Weihua Ji⁶; Joan M Bathon⁷; Jennifer E Van Eyk^{1,2}; ¹*Johns Hopkins University, Baltimore, MD*; ²*Cedars Sinai Medical Systems, Los Angeles, CA*; ³*Beckman Coulter Life Science, Indianapolis, IN*; ⁴*Beckman Coulter, Brea, CA*; ⁵*AB SCIEX, Foster City, CA*; ⁶*National Institute of Standards and Technology, Gaithersburg, MD*; ⁷*Columbia University, New York, NY*
- WP 498 **Secretome Analysis using Label-Free Quantitative Proteomics to Discover Potential Cancer Biomarkers of Benzo(a)Pyrene Exposure;** Marianne Ibrahim¹; Lauriane Kuhn²; Zeina Dagher³; Johana Chicher²; Ramez Chahine⁴; Philippe Hammann²; Emmanuelle Leize-Wagner¹; ¹*LSMIS, CNRS-UMR 7140, University of Strasbourg, Strasbourg, France*; ²*Plateforme Protéomique Strasbourg Esplanade (IBMC), Strasbourg, France*; ³*Equipe Molécules Bioactives, Lebanese University, Beirut, Lebanon*; ⁴*Laboratoire Stress Oxydatif, Lebanese University, Beirut, Lebanon*
- WP 499 **Validation Studies for Serum Biomarkers of Pancreatic Cancer;** Clementina Mesaros^{1,2}; Nathaniel Snyder^{1,2}; Kenneth Yu^{1,3}; Ian A. Blair^{1,2}; ¹*University of Pennsylvania, Philadelphia, PA*; ²*Center for Excellence in Environmental Toxicology, Philadelphia, PA*; ³*Memorial Sloan-Kettering Cancer Center, New York, NY*
- WP 500 **iTRAQ-Based Quantitative Proteomic Analysis of Core-Fucosylated Glycopeptides in Serum of Pancreatic Cancer;** Zhijing Tan; Zhenxin Lin; Song Nie; Haidi Yin; David M. Lubman; *University of Michigan, Ann Arbor, U.S.A*
- WP 501 **High-throughput Analysis of Glycan Variation on Glycoproteins from Serum by the Reverse Lectin-based ELISA Assay and MRM Analysis;** Jing Wu; Jianhui Zhu; Haidi Yin; Ronald Buckanovich; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- WP 502 **Mass Spectrometry Quantitation of sPLA2 Alteration in Human Serum Samples to Investigate Its Proinflammatory Activity;** Vahid Farrokhi¹; Reza Nemat¹; Emily Anstadt²; Frank C. Nichols³; Robert B. Clark²; Xudong Yao¹; ¹*University of Connecticut, Storrs, CT*; ²*University of Connecticut School of Medicine, Farmington, CT*; ³*University of Connecticut School Dental Medicine, Farmington, CT*
- WP 503 **Western Blotting for Post Translational Modifications vs. Quantitative Mass Spectrometry: Study of 3-Nitrotyrosine;** Nadya Galeva; Elena Dremina; Maria Feeney; Christian Schöneich; *University of Kansas, Lawrence, KS*
- WP 504 **Mass Spectrometry (MS) Based Serum Protein Profiling of Depleted and Undepleted Serum;** Santosh Bhosale¹; Robert Moulder¹; Olli Raitakar²; David Goodlett²; Riitta Laheesmaa¹; ¹*University of turku, Turku, Finland*; ²*University of Maryland, Baltimore, MD*; ³*Department of Clinical Physiology and Nuclear Medi, Turku, Finland*
- WP 505 **Rapid Quantitation of Substance P in Plasma using Differential Mobility Spectrometry and Microflow Chromatography;** Daniel Warren; Sushmit Maitra; *AB SCIEX, Framingham, MA*
- WP 506 **Comparison of Different Methods and Informatics Tools for Protein Quantification;** Martha Stapels; Petra Olivova; Monica Lane; Kate Zhang; *Genzyme Corporation, Framingham, MA*
- WP 507 **Quantitative Analysis of Creatinine in Rodent Plasma by Laser Diode Thermal Desorption Coupled to Tandem Mass Spectrometry;** Kristina Gueneva-Boucheva¹; Roger Dinallo¹; Pierre Picard²; ¹*Boehringer Ingelheim, Ridgefield, CT*; ²*Phytronix Technologies Inc., Quebec, Canada*
- WP 508 **Enhanced Laser Ionization Methodology for the Quantitative Analysis of a Biomedically Relevant Analyte;** Logan Miller¹; Steve Shuttleworth²; Matt Pamukcu³; H.M "Skip" Kingston¹; ¹*Duquesne University, Pittsburgh, PA*; ²*Photon Machines Inc., Bozeman, MT*; ³*Applied Isotope Technologies, Pittsburgh, PA*

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WP 509 **LC-MS/MS: A Tool to Mitigate Interferences in Complex Matrices;** Carolyn Burdette; Benjamin Place; Johanna Camara; NIST, Gaithersburg, MD

WP 510 **Liver Mitochondria Proteomics: Protein and PTM Quantitation;** Jenny T.C. Ho¹; Loïc Dayon²; John Corthesy²; Umberto De Marchi²; Antonio Nunez²; Rosa Viner³; Michael Blank³; Steven Danielson³; Madalina Oppermann¹; Martin Hornshaw¹; Andreas Wiederkehr^{2, 4}; Martin Kussmann^{2, 5}; ¹Thermo Fisher Scientific, Hemel Hempstead, UK; ²NIH, Lausanne, Switzerland; ³Thermo Fisher Scientific, San Jose, CA; ⁴Ecole Polytechnique Federale Lausanne, Lausanne, Switzerland; ⁵Aarhus University, Aarhus, Denmark

WP 511 **Targeted Quantitative Proteomics of Protein Biomarkers for Plasma Nutrient Status using Heavy Stable Isotope Labeled Recombinant Proteins;** Raghothama Chaerkady¹; Robert O'Meally¹; Lauren Devine¹; Hee-Sool Rho¹; Jamie L Johnson²; Kerry Schulze²; John D Groopman²; Keith P West²; Robert N Cole¹; ¹Johns Hopkins School of Medicine, Baltimore, MD; ²Johns Hopkins School of Public Health, Baltimore, MD

WP 512 **Targeted Proteomics to monitor Pharmacological Induction of Embryonic Beta Globins in Adult Mice;** Michelle Salemi¹; Hugh Rienhoff²; Brett Phinney¹; ¹UC Davis, Davis, CA; ²Children s Hospital of Oakland, Oakland, CA

WP 513 **Exploring the Detection Limits of ERG Oncoprotein in Prostate Cancer using Different Sample Types Simulating Clinical Specimens;** Jintang He¹; Tujin Shi¹; Athena A. Schepmoes¹; Thomas L. Fillmore¹; Chaochao Wu¹; Albert Dobi²; Shiv Srivastava²; Shyh-Han Tan²; Ahmed A. Mohamed²; Anshu Rastogi²; Jacob Kagan³; Sudhir Srivastava³; Wei-Jun Qian¹; Richard D. Smith¹; Karin D. Rodland¹; Tao Liu¹; David G. Camp¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Center for Prostate Disease Research, Rockville, MD; ³National Cancer Institute, Rockville, MD

WP 514 **Enrichment of EGFR/PI3K/AKT/PEN Proteins using Immunoprecipitation and Analysis with Mass Spectrometry-based Proteomics;** Bhavin Patel; Scott Meier; Kay Opperman; Paul Haney; Barb Kaboord; John C. Rogers; Thermo Fisher Scientific, Rockford, IL

WP 515 **Real-Time Qualitative and Quantitative Analysis of Differentially Expressed Proteins Using a Modified DIA Method;** Tara Schroeder¹; Scott Peterman²; Amol Prakash²; Shadab Ahmad²; Barbara Frewen²; Mary Lopez²; ¹Thermo Fisher Scientific, Somerset, NJ; ²Thermo Fisher Scientific, Cambridge, MA

WP 516 **A High-Throughput, Semi-Automated, Sample Handling Platform for Quantitative Proteomics: A Test-Case Study of Gene Regulation in Mouse Hippocampus;** Paul Piehowski¹; Vladislav Petyuk¹; Arshad Khan²; Anil Shukla¹; Desmond Smith²; Richard D. Smith¹; ¹Pacific Northwest National Lab, Richland, WA; ²UCLA Molecular and Medical Pharmacology Department, Los Angeles, CA

WP 517 **A SISCAPA Immuno-Mass Spectrometric Assay for Quantification of Soluble Transferrin Receptor (sTfR) in Human Serum;** Oliver Drews¹; Rainer Paape¹; Waltraud Evers¹; Morteza Razavi²; Matt Pope²; Leigh Anderson²; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²SISCAPA Assay Technologies, Victoria, Canada

WP 518 **Development of a SISCAPA-MALDI Assay for Multiplexed Analysis of Apolipoprotein A1, Apolipoprotein B and Apolipoprotein E in Human Serum;** Morteza Razavi¹; Irene van den Broek³; Jan Nouta³; Oliver Drews⁴; Detlev Suckau⁴; Rainer Paape⁴; Yuri E.M. van der Burg³; Christa M. Cobbaert³; N. Leigh Anderson¹; Terry W. Pearson^{1, 2}; ¹SISCAPA Assay Technologies,

Washington, DC; ²University of Victoria, Victoria, BC; ³Leiden University Medical Center (LUMC), Leiden, The Netherlands; ⁴Bruker Daltonik GmbH, Bremen, Germany

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WP 519 **Development of a Fast, Sensitive chiral-LC/MS/MS Method for Quantitation of Empagliflozin, a SGLT-2 Inhibitor, and Its Epimer in Human Plasma;** Lin-Zhi Chen¹; Shirin Pagels¹; Steffen Penk²; Michael Wedel²; ¹Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; ²Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany

WP 520 **A Robust and Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Quantification of 24(S)-Hydroxycholesterol in Human Plasma and Cerebrospinal Fluid;** Xuntian Jiang; Rohini Sidhu; Hui Jiang; Jean E. Schaffer; Daniel S. Ory; *Diabetic Cardiovascular Disease Center, Washington, St. Louis, MO*

WP 521 **Comparison of Gas Chromatography and Ultra-performance Liquid Chromatography Coupled with Tandem Mass Spectrometry for Determining Perfluorinated Chemicals;** Yi-Chieh Lai; Chia-Yang Chen; *National Taiwan University, Taipei, Taiwan*

WP 522 **Troubleshooting and Real Time Monitoring of Matrix Effect Generated by Consumable Labware during Ivermectin Quantification by LC-MS/MS;** Mathieu Lahaie; Kevork Mekhssian; Romain Beauvois; Georges Koudssi; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 523 **Post-Column Addition of High pH Solution to Improve Analyte Sensitivity and Avoid On-Column Degradation of Unstable Metabolites in LC-MS/MS;** Julien Nantel; Laurence Mayrand-Provencher; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 524 **Bioanalytical Method for Quantification of Total Apomorphine in Human Plasma by LC-MS/MS;** Melvin Tan; Francesca Ekpo; Erica Hutton; Venetra DeLeon; Edward Wells; Steve Unger; *Worldwide Clinical Trials, Austin, TX*

WP 525 **In Depth Bioanalytical Investigation and Root Cause Analysis of Lamotrigine Severe Degradation in Hemolyzed Plasma Samples by LC-MS/MS;** Nicolaos Soilis; Richard Lavallée; Milton Furtado; Josée Michon; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 526 **Evaluation of Stability of Acyl Glucuronides using LC-MS/MS;** Qingguo Tian; Andreas Grill; Daksha Desai-Krieger; *Forest Laboratories, Inc., Farmingdale, NY*

WP 527 **PPM Level Quantitative Analysis of Genotoxic Impurities in a Pharmaceutical Starting Material;** Meng Xu¹; Catherine Brookes²; Alison Bretnall²; Hongfei Yue¹; John Castoro¹; ¹Bristol-Myers Squibb, New Brunswick, NJ; ²Bristol-Myers Squibb Company, moreton, UK

WP 528 **LC-MS/MS Bioanalysis of Loratadine in DBS Samples Collected by Subjects in a Clinical Study for Assessment of Remote PK Sampling;** Wenkui Li; John Doherty; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*

WP 529 **An Extremely Sensitive LC-MS/MS Method for Quantitation of Fluticasone Propionate (0.4 pg/mL) in Human Plasma;** Xinping Fang; Dawei Zhou; Jinn Wu; *XenoBiotic Laboratories, Inc., Plainsboro, NJ*

WP 530 **Determination of Gangliosides in Human Plasma by a Novel UHPLC/MS/MS Assay;** Qianyang Huang¹; Xiang Zhou¹; Danting Liu¹; Baozhong Xin²; Karen Cechner²; Heng Wang²; Aimin Zhou¹; ¹Cleveland State University, Cleveland, Ohio; ²DDC Clinic, Middlefield, OH

- WP 531 **A Sensitive LC-MS/MS Method for the Quantification of Ethinyl Estradiol and Drospirenone in Human Plasma;** Siddhartha Khurana¹; Naveen Dubey¹; Dhananjay Sharma¹; Sandeep Sharma¹; Anoop Kumar²; Manoj Pillai²; ¹Jubilant Clinsys, Noida, India; ²AB SCIEX DHR holdings India, Gurgaon, India
- WP 532 **In Depth Evaluation of a Novel On-line HybridSPE Technology for Removal of Phospholipids from Protein Precipitation Plasma Samples by LC-MS/MS;** Laurence Mayrand-Provencher¹; Richard Lavallée¹; Milton Furtado¹; David Bell²; Fabio Garofolo¹; ¹Algorithme Pharma Inc., Laval, Canada; ²Sigma-Aldrich, Bellefonte, PA
- WP 533 **Development and Validation of of an Ultra Sensitive UPLC-MS/MS Method for the Determination of Naloxone in Human Plasma;** Xiaohan Cai; Lina Tang; Lan Li; Yuan-Shek Chen; Luca Matassa; *QPS, LLC, Newark, DE*
- WP 534 **Selecting the Right Weighting Factors for Linear and Quadratic Calibration Curves in Bioanalytical LC-MS/MS Assays;** Huidong Gu; Guowen Liu; Jian Wang; Anne Aubry; Mark Arnold; *Bristol-Myers Squibb, Princeton, NJ*
- WP 535 **Impact of Plasma Hemolysis on the Recovery of Phenprocoumon LC-MS/MS Chiral Assay;** Nikolay Youhnovski; Romain Beauvois; Mathieu Lahaie; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 536 **Oral Fluid Testing for Buprenorphine and THC by “Dilute and Shoot” LC-MS/MS;** Jeffrey Enders; Ayodele Morris; Gregory Mcintire; *Ameritox, Ltd, Greensboro, NC*
- WP 537 **Development and Qualification of an UPLC-MS/MS Method for Simultaneous Determination of Five Isomeric Analytes (potential metabolites) in Human Plasma;** Yu-Luan Chen¹; Shoko Ochiai²; Estela Skende¹; Julie Tollefson³; Amber LaFayette³; ¹Sunovion, Inc., Marlborough, MA; ²Dainippon Sumitomo Pharma, Osaka, Japan; ³Covance, Madison, WI
- WP 538 **Parallelism Comparison between Surrogate and Biological Matrix for the Quantification of Endogenous Levels using Surrogate Matrix Calibration Curve by LC-MS/MS;** Richard Lavallée; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 539 **A Fast and Simple LCMSMS Derivatization Approach towards Quantification of Low Molecular Weight Compounds of Molecular Weight Less than 100Da;** Mohan Kasi¹; Arvind Thyagarajan²; Saravanan Subramaniyan²; Rampriya Uthayakumar²; Raman Palvannanathan²; Govindarajan Chandramohan²; Venkat Manohar²; Devadasan Velmurugan¹; ¹Dept. of CAS in Crystallography & Biophysics, University of Madras, Chennai, India; ²IICMS, Chennai, India
- WP 540 **Simultaneous Quantitation of Nebivolol and Valsartan in Human Plasma;** Mei Li; Hongzhi Liu; Helen Deng; Anita Dalko; Surya Kandukuri; Nicola Hughes; *Bioanalytical Laboratory Services (LifeLabs), Toronto, Canada*
- WP 541 **Quantitative Measurement of Ultra-low Level of Tiotropium Bromide in Human Plasma using Two-Dimensional Liquid Chromatography (2D-LC) and Tandem Mass Spectrometry;** Jingduan Chi; Melissa Meyer; Fumin Li; *PPD Inc, Madison, WI*
- WP 542 **A Study of the Electrospray/Mass Spectral Characteristics of De-Protonated Molecular and Chloride Adduct Ions of Phenicols: Implications in Quantitative Analysis;** Kwenga Sichilongo; *University of Botswana, Gaborone, Botswana*
- WP 543 **The Bioanalysis of Propylparaben, a Suspected Environmental Estrogenic Agent, by LC-MS/MS;** Yue Zhao; Guowen Liu; Hongwu Shen; lakshmi Sivaraman; Anne-Francoise Aubry; Mark Arnold; Jim Shen; *Bristol-Myers Squibb Co., Princeton, NJ*
- WP 544 **Evaluation of the Budesonide 22R and 22S Epimers Fragmentation in LC-MS/MS and its Impact in Quantitative Bioanalysis;** Eugénie-Raphaëlle Bérubé; Sylvain Latour; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 545 **How to Prevent Changes in Plasma Integrity and its Impact on LC-MS/MS Bioanalysis Due to Organic Solvent and Storage Conditions;** Romain Beauvois¹; Silvana Olivieri²; Milton Furtado¹; Fabio Garofolo¹; ¹Algorithme Pharma Inc., Laval, Canada; ²ACRAF – Angelini Research Center, S. Palomba, Pomezia, Rome, Italy
- WP 546 **Quantitation of Budesonide in Human Plasma: Improved Sensitivity Using Acetate Adduct Ion;** HongZhi Liu; Mei Li; Rizwan Muhammad; Jenny Shen; Surya Kandukuri; Anita Dalko; Nicola Hughes; *Bioanalysis Laboratory Services (LifeLabs), Toronto, Canada*
- WP 547 **Challenges in Developing a Ten Analyte Statin HPLC-MS/MS Assay in Multiple Rat Matrices;** Ryan Lutz; Cynthia M. Chavez-Eng; Dina Goykhman; Kevin Bateman; *Merck & Co., West Point, PA*
- WP 548 **A Highly Specific Pre-Charged Triphenylphosphine-Based Derivatization Agent for Trace-Level Detection of Ethinylestradiol;** Lucie Loukotkova¹; Priyanka Chitranshi¹; Gordon Surratt²; Goncalo Gamboa da Costa¹; ¹FDA/NCTR, Jefferson, AR; ²Waters Corp., Milford, MA
- WP 549 **Large-Scale Retrospective Evaluation of Regulated LC-MS Bioanalysis Projects Using Different Total Error Approaches;** Aimin Tan¹; Taoufiq Saffaj²; Adrien Musuku³; Kayode Awaie¹; Bouchaib Ihssane²; Fayçal Jhila²; Saad. Alaoui Sosse²; Fethi Trabelsi¹; ¹BioPharma Services Inc., Toronto, Canada; ²Université Sidi Mohamed Ben Abdallah, Fès, Morocco; ³Pharmascience Inc., Montreal, Canada
- WP 550 **A Novel Microflow UPLC-MS/MS Multiplexed Assay for the Absolute Quantitation of Thyroid Hormones in Serum;** Hend Ibrahim; Lisa Wolfe; Corey Broeckling; Jessica Prenni; Jessica Prenni; *Colorado State University, Fort Collins, CO*
- WP 551 **Evaluation of Integrated Microfluidic Device device for targeted small molecule bioanalysis;** Aaron Ledvina; *Covance Laboratories Inc., Madison, WI*
- WP 552 **Quantitation of Aminoglycosides in Pharmaceutical Preparations by ESI-MS without the Need of Chromatographic Separation or Derivatization;** Freneil B. Jariwala; John A. Hibbs; Iryna Zhuk; Svetlana A. Sukhishvili; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- WP 553 **Using HPLC-MS to Assess Host-Mediated Conversion of Pyrazinamide to Pyrazinoic Acid Across Species;** Matthew Zimmerman; Xiaohua Li; Brendan Prideaux; Jansy Sarathy; Veronique Dartois; *Public Health Research Institute, Rutgers, Newark, NJ*
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- WP 554 **Study of Cyanobacterial Microcystins using High Performance Tandem Mass Spectrometry;** Yulin Qi; Stella Bortoli; Dietrich Volmer; *Saarland University, Saarbrücken, Germany*
- WP 555 **Stercobilin Detection and Quantification in Public Swimming Facilities: Method Development for Low and High Resolution Mass Spectrometry;** Heather L. Rudolph; Troy Wood; *SUNY University at Buffalo, Buffalo, NY*

- WP 556 **Screening of Polymer Additives in Drinking Water Stored in PET Bottles by UHPLC-ESI-IT-TOF MS;** Mustafa Yilmaz; Hamdi TEMEL; DUBTAM, Dicle University, Diyarbakir, Turkey
- WP 557 **Environmental Forensic Investigation of PAHs: Determination and Apportionment of Possible Sources;** Ashley Gates¹; Jack Cochran²; Melinda Pham¹; Frank Dorman¹; ¹Penn State University, State College, PA; ²Restek, Bellefonte, PA
- WP 558 **Sensitive and Accurate LC-MS/MS Assay of Perfluorinated Compounds in Water;** Hui Qiao; Joshua Sha Ye; Changtong Hao; IONICS Mass Spectrometry Group Inc, Bolton, Canada
- WP 559 **Non-targeted Analysis Phase II Metabolites in Surface water using Full Scan Tandem Quadrupole Mass Spectrometry;** Matthew Reichert; Piotr Krolikowski; M. Paul Chiarelli; Loyola University, Chicago, IL
- WP 560 **Determination of Endocrine Disrupting Chemicals in Drinking Water at Sub ng/L Levels Using Direct Injection and Triple Quadrupole Mass Spectrometry;** Dorothy Yang¹; László Tölgyesi²; Bernhard Wuest³; Anabel Fandino⁴; ¹ Santa Clara, CA; ²Agilent Technologies Sales & Services GmbH & Co. K, Waldbronn, Germany; ³Agilent Technologies GmbH, Waldbronn, Germany; ⁴Agilent Technologies, Santa Clara, CA
- WP 561 **Direct Injection LC-MS/MS Determination of Acesulfame and Sucralose for Monitoring of Water Quality;** Minghuo Wu; Yichao Qian; Xing-Fang Li; University of Alberta, Edmonton, Canada
- WP 562 **Occurrence and Toxicity of Haloacetaldehydes in Drinking Waters: Discovery of Iodo-Acetaldehyde as a Drinking Water Disinfection By-Product;** Susan Richardson¹; Cristina Postigo^{2,4}; Clara Jeong³; Elizabeth Wagner³; Jane Ellen Simmons²; Michael Plewa³; Damia Barcelo⁴; ¹University of South Carolina, Columbia, SC; ²U.S. EPA, NHEERL, RTP, NC; ³University of Illinois, Urbana, IL; ⁴Spanish National Research Council, Barcelona, Spain
- WP 563 **Determination of Unknown Chlorinated Water Pollutants in the Chicago River;** Qian Wang¹; Kathryn M. Renyer²; M. Paul Chiarelli¹; ¹Loyola University, Chicago, IL; ²Morehead St. University, Morehead, KY
- WP 564 **High Resolution/Accurate Mass (HR/AM) Detection of Anatoxin-a in Lake Water Using LDTD-APCI Coupled to a Q-Exactive Mass Spectrometer;** Audrey Roy-Lachapelle¹; Morgan Sollicet¹; Christian Deblois²; Marc Sinotte³; ¹Université de Montréal, Montréal, Canada; ²MDDEFP, CEAEQ, Québec, Canada; ³MDDEFP, DSEE, Québec, Canada
- WP 565 **Ultra-fast LDTD-APCI-MS/MS Analysis of Estrogens in Chlorinated Drinking Water and the Impact of Bromide on the Oxidation Kinetics;** Sung Vo Duy¹; Paul Fayad¹; Michèle Prévost²; Sébastien Sauvé¹; ¹Université de Montréal, Montreal, QC, Canada; ²École Polytechnique de Montréal, Montreal, QC, Canada
- WP 566 **The Use of Chemometrics and High Resolution Accurate Mass GC/Q-TOF in the Identification of Environmental Pollutants in Wastewater Effluents;** Anthony Gravel¹; Praveen Kuty¹; Sofia Aronova²; Jennifer Gushue²; Terry Sheehan²; ¹Natural Resources Wales, Wales, UK; ²Agilent Technologies, Inc., Santa Clara, CA
- WP 567 **HPLC-MS/MS Investigation of Halo-hydroxylbenzoquinones as Stable Haloquinone Disinfection By-Products in Treated Water;** Wei Wang; Yichao Qian; Steve Hrudev; Xing-Fang Li; University of Alberta, Edmonton, Canada
- WP 568 **Investigation of Suspected and Unknown Micropollutants and Transformation Products from a Waste Water Treatment Plant with Full Scale Ozonation;** Christoph Portner¹; Olaf Scheibner²; Sebastian Westrup³; Jochen Tuerk¹; ¹Institute of Energy and Environmental Technology, Duisburg, Germany; ²Thermo Fisher Scientific, Bremen, Germany; ³Thermo Scientific, Dreieich, Germany
- WP 569 **Determination and Removal of N-Nitrosamine Precursors in Drinking Water System;** Honglan Shi¹; Qihua Wu¹; Yinfa Ma¹; Craig Adams²; Hua Jiang³; ¹Missouri S&T, Rolla, MO; ²Utah State University, Logan, UT; ³City of Tulsa Water and Sewer Department, Tulsa, OK
- WP 570 **Environmental Forensics of Wastewater Samples for Determination of Emerging Contaminants;** Adrienne Brockman¹; Dr. Frank Dorman¹; Jack Cochran²; Michelle Misselwitz²; ¹ University Park, PA; ²Restek, Bellefonte, PA
- WP 571 **Dioxin in Drinking Water by One-Step Solid Phase Extraction;** Hamid Shirkhan; Tom Hall; Fluid Management Systems, Watertown, MA
- WP 572 **EPA 625: Base, Neutral, Acid Semi-Volatiles in Municipal and Industrial Waste Water by SPE;** Philip GERMANSERFER; Lawrence Kramer; Fluid Management Systems, Watertown, MA
- WP 573 **Automated Low Background Solid Phase Extraction System for Perfluorinated Compounds from Water;** Phil Bassignani; Fluid Management Systems, Inc., Watertown, MA
- WP 574 **Organic Extract Analysis by in-Line Dilution Reversed-Phase LC-MS/MS;** Brent McKay Allred¹; Mathew Perkins¹; Johnsie Lang²; Morton Barlaz²; Jennifer Field¹; ¹Oregon State University, Corvallis, Oregon; ²North Carolina State University, Raleigh, NC
- WP 575 **Strategies and Techniques for Identifying Unknown Compounds in Environmental Samples;** Eric J. Reiner¹; Karl J. Jobst¹; Miren Pena-Abaurrea²; Anne L. Myers²; Li Shen¹; Alina Muscalu¹; Ralph Ruffolo¹; Vince Y. Taguchi¹; Paul A. Helm¹; ¹Ontario Ministry of the Environment, Toronto, Canada; ²University of Toronto, Toronto, Canada
- WP 576 **Analysis of Electronics Waste by 2D-GC Combined with High-Resolution Mass Spectrometry: Using Exact Mass Information to Explore the Data;** Masaaki Ubukata¹; Karl J. Jobst²; Eric J. Reiner²; Stephen Reichenbach³; Qingping Tao⁴; Jiliang Hang⁴; Zhanpin Wu⁵; A. John Dane¹; Robert B. Cody¹; ¹JEOL USA, INC., Peabody, MA; ²Ontario Ministry of the Environment, Toronto, Canada; ³University of Nebraska-Lincoln, Lincoln, NE; ⁴GC Image LLC, Lincoln, NE; ⁵Zoex Corporation, Houston, TX
- WP 577 **Non-Targeted Analysis of Environmental Contaminants in Northern Fur Seals Using Comprehensive Two-Dimensional Gas Chromatography Time-of-Flight Mass Spectrometry;** Jacolin Murray¹; Benjamin Place¹; Natalie Rosenfelder²; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²Chemical and Veterinary Investigations Office, Stuttgart, Germany
- WP 578 **Persistent Organic Pollutants in Serum using Pressurized Liquid Extraction, Multi-Column Clean Up and Concentration;** Tom Hall; Rudolf Addink; Fluid Management Systems, Watertown, MA
- WP 579 **Oklahoma Fish Kill Study: Looking for a Toxic Needle in an Environmental Haystack;** Tammy Jones-Lepp¹; Wayne Sovocool²; Don Betowski¹; Patrick DeArmond³; Vince Taguchi⁴; Charlita Rosal¹; ¹USEPA/ORD/NERL-ESD, Las Vegas, NV; ²retired USEPA, Henderson, NV; ³former USEPA post-doctoral Fellow, Las Vegas, NV; ⁴Ministry of the Environment-Ontario, Toronto, Canada

- WP 580 **Determination of Alkylphenol Ethoxylate in Textiles and Leathers by NPLC and Quadrupole Orbitrap MS; Nam-Yong Cheong¹; Bruce Lee¹; Su-Jin Eo¹; Yoon-Suk Lee²; Seoung-Woon Myung³; ¹KATRI, An-Yang, Korea; ²Euro Science, Seong-Nam, Korea; ³Kyonggi University, Su-Woon, Korea**
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- WP 582 **A Steroidomics Approach to Detect the Misuse of Oral Anabolic Steroids in Equine Sports by Biomarkers Profiling; George H.M. Chan; Emmie N.M. Ho; Terence S.M. Wan; *Racing Laboratory, The Hong Kong Jockey Club, Sha Tin, N. T., Hong Kong, China***
- WP 583 **Metabolomics Investigation of Spiked Compound Differences in Human Plasma; Amrita Cheema¹; John M Asara²; Thomas Neubert³; Chris Turck⁴; ¹Georgetown University, Washington, DC; ²Beth Israel Deaconess Medical Center, Boston, MA; ³Skirball Institute, NYUMC, New York, NY; ⁴Max Planck Institute of Psychiatry, Munich, Germany**
- WP 584 **Development, Quantitative Evaluation and Application of a High Resolution Metabolomics Technology using HILIC Chromatography Coupled to a Q-Exactive Mass Spectrometer; Xiaojing Liu; Alexander Shestov; Jason Locasale; *Cornell University, Ithaca, NY***
- WP 585 **Gas Chromatography-Mass Spectrometry Analysis of Human Mesenchymal Stem Cell Metabolism during Proliferation and Osteogenic Differentiation under Different Oxygen Tensions; Nathalie Munoz; Yijun Liu; Timothy Logan; *FSU, Tallahassee, Florida***
- WP 586 **Ion Mobility-derived Collision Cross-Sections Databases for Metabolomics and Lipidomics; Giuseppe Paglia¹; Jonathan P. Williams²; Lochana Menikarachchi³; J. Will Thompson⁴; Hernando Olivos⁵; Steven Lai⁶; Richard Tyldesley-Worster⁶; Arthur Moseley⁶; David Grant³; James Langridge⁶; Bernhard O. Palsson⁷; Giuseppe Astarita⁵; ¹Center for Systems Biology, University of Iceland, Reykjavik, Iceland; ²Waters, Manchester, N/A; ³University of Connecticut, Storrs, CT; ⁴Duke University School of Medicine, Durham, NC; ⁵Waters, Milford, MA; ⁶Duke University School of Medicine, Durham, NC; ⁷Systems Biology Research Group, UCSD, San Diego, CA**
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- WP 588 **Myth Busters: The Truth About Metabolomics And Gas Chromatography-High Resolution Time-of-Flight Mass Spectrometry; David Alonso¹; Joe Binkley¹; Lorne Fell²; ¹Leco Corporation, St. Joseph, MI; ²Leco, St Joseph, MI**
- WP 589 **Development of a Plant, Algae, and Microbial Metabolomics Research Coordination Network and US Chapter of the Metabolomics Society; Lloyd W. Sumner¹; Oliver Fiehn²; Georg Jander³; James C. Liao⁴; Basil Nikolau⁵; ¹The Samuel Roberts Noble Foundation, Ardmore, OK; ²University of California, Davis, Davis, CA;**
- ³Boyce Thompson Institute for Plant Research, Ithaca, NY; ⁴University of California, Los Angeles, Los Angeles, CA; ⁵Iowa State University, Ames, IA
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- WP 592 **Metabolomics Technology Validated Quality Markers for Biobank Plasma Samples; Michael Herold¹; Beate Kamlage¹; Oliver Schmitz¹; Philipp Schatz²; ¹metanomics GmbH, Berlin, Germany; ²Metanomics Health GmbH, Berlin, Germany**
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- WP 594 **Direct Mitochondrial Metabolites Detection in a HepG2 Cell by Live Single-cell Mass Spectrometry; Tsuyoshi Esaki; Sachiko Date; Hajime Mizuno; Ai Fujita; Tsutomu Masujima; *Quantitative Biology Center (QBiC), RIKEN, Suita, Osaka, Japan***
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- WP 597 **Characterization of HILIC Columns with Zwitterionic Functional Groups: Correlation between Retention, Selectivity, Stationary Phase and Water Layer Thickness; David Lentz²; Tobias Jonsson¹; Phuoc Dinh³; Patrik Appelblad¹; Wen Jiang¹; ¹Merck Millipore, Darmstadt, Germany; ²EMD Millipore, Billerica, MA; ³Umea University, Umea, Sweden**
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- WP 601 **Disruption of Amino Acid Metabolism in Radiation-Induced Lung Injury;** Fei Li¹; Jace Jones¹; Gregory Tudor²; Catherine Booth²; Thomas MacVittie³; Maureen Kane¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD; ²Epistem Ltd, Manchester, UK; ³University of Maryland, School of Medicine, Baltimore, MD
- WP 602 **Multioomic Profiling of Acute Immune Response in an SIV Macaque Model of HIV-AIDS;** Ravi Tharakan¹; Anne Blackwell²; Ceereena Ubaida Mohien¹; David Colquhoun³; Brigitte Simons⁴; David Graham¹; ¹JHU, Baltimore, MD; ²Agilent Technologies, Wilmington, DE; ³Shimadzu Scientific Instruments, Columbia, MD; ⁴AB SCIEX, Montreal, QC
- WP 603 **Metabolomic and Lipidomic Analyses of Diet-Induced Inhibition of Hepatic De Novo Lipogenesis with Carbohydrate Restriction;** Daniela M Schlatter¹; Michelle A Puchowicz¹; Giovanni Pallante²; Tim Stratton²; Mark R Chance¹; Junhua Wang²; ¹Case Western Reserve University, Cleveland, OH; ²Thermo Fisher Scientific, San Jose, CA
- WP 604 **MRMPROBS Suite: Metabolomics Software for Large-Scale Multiple Reaction Monitoring Assays;** Hiroshi Tsugawa^{1,2}; Mitsuhiro Kanazawa³; Atsushi Ogiwara³; Masanori Arita^{1,4}; ¹RIKEN, Yokohama, Japan; ²Osaka Univ, Osaka, Japan; ³Reifys, Inc., Minato-ku, Japan; ⁴NIG, Mishima, Japan
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- WP 608 **In vivo Stable Isotope Labeling of ¹³C and ¹⁵N Labeled Metabolites and Lipids;** Susanne Breilkopf¹; Min Yuan¹; Costas Lyssiotis³; John M Asara^{1,2}; ¹Beth Israel Deaconess Medical Center, Boston, MA; ²Harvard Medical School, Boston, MA; ³Weill Cornell Medical College, New York, NY
- WP 609 **Protocol for Determination of Redox and Bioenergetics Molecules in Tissue Samples using Tandem Mass Spectrometry and Zwitterionic HILIC Columns;** Hardik Shah; Albert Einstein College of Medicine, Bronx, NY
- WP 610 **Development and Application of a UPLC/MRM-MS Method for the Comprehensive Analysis of >50 Bile Acids in Human and Mouse Samples;** Jun Han¹; Yang Liu¹; Renxue Wang²; Victor Ling²; Christoph Borchers^{1,3}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²BC Cancer Agency, University of British Columbia, Vancouver, Canada; ³UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 611 **3-Nitrophenylhydrazine as an Efficient Chemical Derivatization Reagent in LC/MS-Based Quantitative Metabolomics;** Jun Han¹; Karen Lin¹; Carita Sequeria¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 612 **LC/MS Response Factor Dependence on Mobile Phase Composition using newly Authenticated Acylsugar Metabolites;** Banibrata Ghosh; Zhenzhen Wang; A. Daniel Jones; Michigan State University, East Lansing, MI
- WP 613 **Simultaneous Analysis of Primary Metabolites by Triple Quadrupole LC/MS/MS using Pentafluorophenylpropyl Column;** Tsuyoshi Nakanishi; Shimadzu Corporation, Kyoto, Japan
- WP 614 **Parallel UHPLC-MS/MS System for High-Speed SRM Quantification using Fast Electrospray Polarity Switching;** Kyoko Watanabe^{1,2}; Emmanuel Varesio¹; Neil Loftus³; Gerard Hopfgartner¹; ¹University of Geneva, University of Lausanne, Geneva, Switzerland; ²Shimadzu Corporation, Kyoto, Japan; ³Shimadzu Corporation, Manchester, UK
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- WP 618 **Human rCYP Phenotyping as a Model Experiment for Combination of Qualitative and Quantitative HRMS Data in Drug Discovery;** JianHua Liu¹; Veronica Zelesky¹; Carrie Funk²; Nathaniel Woody²; John Janiszewski¹; Ismael Zamora³; Eva Duchoslav⁴; ¹Pfizer Inc., Groton, CT; ²Pfizer, Groton, CT; ³Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; ⁴AB Sciex, Concord, ON
- WP 619 **Simultaneous Metabolic Stability Determination and Metabolite Identification Using Q Exactive System;** Ruiqing Qiu; Gang Luo; Covance, Madison, WI
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- WP 621 **Development of a Quantitative LCMS Method for the Novel Antifungal Compound Occidiofungin using TraceFinder 3.1 with Intelligent Sequencing;** Jamie K Humphries; Thermo Electron, Keller, TX
- WP 622 **An Integrated Process for Metabolite Based in vitro Reaction Phenotyping in Early Discovery using LC/HRMS;** Jonathan L. Josephs¹; Emily Luk¹; Mary Grubb¹; Yanou Yang¹; William Humphreys²; ¹Bristol-Myers Squibb, Pennington, NJ; ²Bristol-Myers Squibb, Lawrenceville, NJ
- WP 623 **Rapid LC-MS/MS Determination of Digoxin and Digitoxin with Minimal Matrix Effects;** Xiaoning Lu; David S. Bell; Sigma-Aldrich, Bellefonte, PA
- WP 624 **Determination of β -blockers from Human Plasma with SPE 96-well Plate Format and LC-MS/MS;** Ruyi Wang¹; Guotao Lu²; ¹Bonna Agela Technologies Ltd., Tianjin, China; ²Bonna Agela Technologies Inc, Wilmington, DE
- WP 625 **The Application of UHPLC and Ultrafast-LCMSMS to the Analysis of Small Volume Biological Samples for Drug Residues;** Paul Wynne¹; Bruce Fraser²; John Hewetson³; Nigel Grieves³; ¹Shimadzu, Park Orchards, Australia;

²Shimadzu Scientific Instruments (Oceania), Palmerston North, New Zealand; ³Shimadzu Australasia, Sydney, Australia

WP 626 **Strategy for Predicting Molecular Coverage and Enhancing Successful Analysis for CACO2 Studies in High-Throughput LDTD-MS/MS;** Pierre Picard; Serge Auger; Alex Birsan; Sylvain Letarte; Jean Lacoursiere; *Phytronix Technologies, Inc., Quebec, Canada*

WP 627 **The ADME-Hub: Formalizing and Automating Information Flow in the Preparation and Measurement of Lead Optimization Assays;** Wayne Lootsma¹; Steven Ainley¹; Nick Levitt²; Brendon Kapinos³; Veronica Zelesky³; John Janiszewski³; ¹Sound Analytics, LLC, Niantic, CT; ²TwoCenter Technologies, Cambridge, MA; ³Pfizer Inc., Groton, CT

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WP 628 **Accelerated and Robust Monitoring for Immunosuppressants using Triple Quadrupole Mass Spectrometry;** Natsuyo Asano; Tairo Ogura; Kiyomi Arakawa; *Shimadzu corporation, Kyoto, Japan*

WP 629 **Development of a Sensitive Liquid Chromatography-Tandem Mass Spectrometric Method for Pharmacokinetic Study of Telbivudine in Human Plasma;** Bicui Chen¹; Bin Wang¹; Xiaojin Shi¹; Yuling Song²; Changkun Li²; Qian Sun²; Jinting Yao²; Taohong Huang²; Kawano Shin-ichi²; Hashi Yuki²; ¹Pharmacy Department, *Huashan Hospital, Shanghai, China*; ²Shimadzu (China) Co., Ltd, *Shanghai, China*

WP 630 **Application of In-Source Fragmentation in More Accurate Metabolite Semi-quantification by Peak Area from High-Resolution Mass Spectrometry;** Lin Chen; Xinping Fang; Jinn Wu; Li-Quan Wang; *XenoBiotic Laboratories, Inc, Plainsboro, NJ*

WP 631 **UPLC Coupled with High Resolution Mass Spectrometry for Un-biased MS Scanning and Data Banking for Metabolite Exposure Comparison across Species;** Hongying Gao; R. Scott Obach; *Pfizer, Inc, Groton, CT*

WP 632 **Mass Spectrometric Pharmacokinetics and Pharmacodynamics Analysis of Drugs on Three-Dimensional (3-D) Cell Cultures in a 3-D Printed Microfluidic Device;** Xin Liu¹; Sarah Y. Lockwood²; Amanda B. Hummon¹; Dana M. Spence²; ¹University of Notre Dame, *Notre Dame, Indiana*; ²Michigan State University, *East Lansing, MI*

WP 633 **Quantitation of Insulin Analogue Glargine and Its Two Metabolites M1 and M2 with LC-MS/MS for Dog Toxicokinetics Study;** Yong-Xi Li¹; Yan Ke¹; Junyu Li¹; Run Li²; Xiaofeng Chen²; Sahana Mollah³; Xu Wang³; ¹Medpace, *Cincinnati, OH*; ²HEC Pharma Co. Ltd, *Guangdong, China*; ³AB SCIEX, *Framingham, MA*

WP 634 **Acyl Glucuronides Separation Method for Plasma Analysis by LDTD-MS/MS in Less than 9 Seconds per Sample;** Jean Lacoursiere; Alex Birsan; Serge Auger; Sylvain Letarte; Pierre Picard; *Phytronix Technologies Inc., Quebec, Canada*

WP 635 **Investigating Biological Variation in Human Hepatocytes of Phase I and II drug Metabolism Enzymes;** Xu Wang¹; Hui Zhang²; Christie Hunter³; ¹AB SCIEX, *Framingham, MA*; ²Pfizer, *Groton, CT*; ³AB SCIEX, *Redwood City, CA*

WP 636 **Overcoming Metabolite Interferences in Measuring Absolute Oral Bioavailability using Intravenous Microdosing of ¹⁴C-Labeled Drug and Accelerator Mass Spectrometry (AMS);** Naiyu Zheng¹; Jianing Zeng¹; Michael Furlong¹; Xiaolu Tao¹; Stephen Dueker²; Van Ly¹;

Daisie Chiuu²; Wesley Turley¹; John Easter¹; Ishani Savant¹; Anne-Françoise Aubry¹; Mark E. Arnold¹; ¹Bristol-Myers Squibb Company, *Princeton, NJ*; ²Eckert & Ziegler Vitalea Science, *Davis, CA*

WP 637 **Achieving Maximum Sensitivity for Drug Metabolism and Bioanalytical Workflows: Investigating Time-Of-Flight and Ion Mobility Modes of Acquisition;** Mark Wrona; Craig Dorschel; Yun Aleyunas; Kevin Cook; Stephen McDonald; Paul Rainville; *Waters, Milford, MA*

WP 638 **Capillary Microsampling (CMS) of Whole Blood for Drug Discovery Studies in Mice: An Alternative to DBS Sampling in Bioanalysis;** Walter Korfmacher¹; Maria Fitzgerald¹; Yongyi Luo²; Stacy Ho¹; Jie Wang²; Zhongtao Wu²; Richard Knapp²; Gregory Snow³; Tom O'Shea¹; ¹Genzyme, *Waltham, MA*; ²Sanofi, *Waltham, MA*; ³Agilux Laboratories, *Worcester, MA*

WP 639 **Fast and Sensitive Quantitation of Substrates of Hepatic Uptake Transporters in Cells: Paradim Shift from Radioactivity Detection to LC/MS Analysis;** Ming Yao; Hong Shen; Weiping Zhao; Yong-Hae Han; Praveen Balimane; W. Griff Humphreys; Mingshe Zhu; *Bristol-Myers Squibb, Princeton, NJ*

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WP 641 **Next Generation Plasma Collection Technology for the Clinical Analysis of Temozolomide by HILIC/MS/MS;** Alan J Barnes¹; Adam McMahon²; Neil J Loftus¹; ¹Shimadzu, *Manchester, UK*; ²WMIC, *University of Manchester, Manchester, UK*

WP 642 **Investigation of Solid Phase Micro Extraction as an Alternative to Dried Blood Spot;** Craig Aurand; David Bell; Robert Shirey; Emily Barrey; *Sigma Aldrich, Bellefonte, PA*

WP 643 **Determination of Drugs in Blood Samples by Automatic SPE Apparatus Coupled with Gas Chromatography-Mass Spectrometry;** Xiaoyan Cao; Guotao Lu; *Bonna-Agela, Tianjin, China*

WP 644 **Dried Plasma Spots Derived from Filtered Whole Blood. Hemato-compatible?;** Robert Sturm¹; Jack Henion¹; Richard Abbott²; Phillip Wang³; ¹Quintiles, *Ithaca, NY*; ²Shire, *Hampshire, UK*; ³Shire, *Wayne, PA*

WP 645 **Evaluation of Plasma Microsampling for Dried Plasma Spots (DPS) in Quantitative LC-MS/MS Bioanalysis using Ritonavir as a Model Compound;** Wenkui Li; John Doherty; Sarah Favara; Christopher Breen; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*

WP 646 **A Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Quantitative Analysis of Efavirenz, Emtricitabine and Tenofovir in Human Dried Blood Spots;** Praveen Srivastava; Jeffrey Barrett; Athena Zuppa; Ganesh Moorthy; *CHOP, Philadelphia, PA*

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- WP 648 **Quantitation of Underivatized Tetrahydrocannabinol (THC) in Dry Blood Spots by a Highly Sensitive LC-MS/MS Instrument**; Sha Joshua Ye; Mitesh Patel; Hui Qiao; Ellie Majdi; *IONICS Mass Spectrometry Grp, Bolton, Canada*
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- WP 650 **High Resolution, Accurate Mass Screening of Anesthetic Compounds and Their Metabolites in Urine by Paper-Spray Q Exactive Mass Spectrometry**; Maria C. Prieto Conaway¹; Tim Stratton¹; Hans Gensemann²; Caroline Ding¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Bremen, Germany*
- WP 651 **Automated Analysis of Dried Blood, Plasma and Urine Samples by Flow-Through Desorption Coupled to Online SPE and Mass Spectrometry**; Lena Knecht; Emile Koster; Cornelis Tump; *Spark Holland, Emmen, Netherlands*
- WP 652 **Application of Dried Blood Spot Technology for Quantitation of the Glucan Synthesis Inhibitor MK-3118 (SCY-078) in Human Blood by LC-MS/MS**; Huizhi Xie; Yang Xu; Lingling Xue; Sheng Bi; Michael Schwartz; Cindy Miller-Stein; Wei Xie; Wendy Comisar; Evan Friedman; Michele Trucksis; Sheila Breidinger; Eric Woolf; *Merck & Co., West Point, PA*
- WP 653 **Identification of Metabolites of Harmine in Rat Plasma using HPLC-Trap-MS-MS**; Shuang Zhao; Beibei wang; Peng Tan; Liu Yonggang; *, Beijing, China*
- WP 654 **Multiplexed MRM-based Protein Quantification in Dried Blood Spot Samples**; Andrew Chambers¹; Andrew Percy¹; Juncong Yang¹; Christoph Borchers^{1,2}; ¹*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; ²*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*
- WP 655 **Determination of Psychosine and Glucopsychosine in Dried Blood Spots by LC-MS/MS for Krabbe and Gaucher Diseases**; Coleman Turgeon¹; Joseph Orsini²; Mark J. Magera¹; Dimitar Gavrilov¹; Devin Oglesbee¹; Kimiyo Raymond¹; Silvia Tortorelli¹; Piero Rinaldo¹; Dietrich Matern¹; ¹*Biochemical Genetics Laboratory, Mayo Clinic, Rochester, MN*; ²*New York State Dept of Health, Wadsworth Center, Albany, NY*
- WP 656 **Clinical Diagnostics of Neuronal Ceroid Lipofuscinoses on Dry Blood Spots by Fluorimetry and MRM-MS using New Coumarin-based Substrates**; Michael Przybylski¹; Claudia Cozma¹; Marius Iurascu¹; Thomas Braulke²; Angela Schulz²; ¹*Universitat Konstanz, Konstanz, Germany*; ²*University Medical Center Hamburg-Eppendorf, Hamburg, Germany*
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- WP 657 **Use of Multivariate Curve Resolution and Ion Mobility-Mass Spectrometry for Isomer Differentiation**; Behrooz Zekavat¹; Brett Harper¹; Matthew Brantley²; Michael E. Pettit¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*; ²*University of Texas at Tyler, Tyler, TX*
- WP 658 **Energy Resolved Ion Mobility Deconvolution of Isobaric Mixtures**; Brett Harper¹; Behrooz Zekavat¹; Matthew Brantley²; Michael Pettit¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*; ²*University of Texas at Tyler, Tyler, TX*
- WP 659 **Development of Relative Ion Mobility and Molecular Modeling (RIM3) as a Novel Approach to Metabolite Structural Identification**; Sean Yu; Ian Mcintosh; Deping Wang; Dan Cui; *Merck & Co, West Point, PA*
- WP 660 **Elucidation of Gramicidin A Conformational Preferences Utilizing Ion Mobility Mass Spectrometry**; John Patrick¹; David H. Russell²; ¹*Texas A&M, College Station, TX*; ²*Texas A&M University, College Station, TX*
- WP 661 **Evolution of Hydrogen Bond Networks in Protonated Water Clusters H⁺ (H₂O)_n (n = 1-150) Studied by Cryogenic Ion Mobility-Mass Spectrometry**; Kelly A. Servage; Joshua A. Silveira; Kyle L. Fort; David H. Russell; *Texas A&M University, College Station, TX*
- WP 662 **Displacement of Metal Ions from Metallothionein using N-ethylmaleimide: Kinetics and Effect of Covalent Labeling on Conformation**; Shu-Hua Chen; Liuxi Chen; David H. Russell; *Texas A&M University, College Station, TX*
- WP 663 **Analysis of Ions Generated From Native Spray Conditions with Trapped Ion Mobility Spectrometry (TIMS)**; Mark Ridgeway; Joshua Silveira; Jacob Meier; Melvin A. Park; *Bruker Daltonics, Inc., Billerica, MA*
- WP 664 **Temperature-Dependent Conformer State Distributions of Model Peptides in Trapped Ion Mobility Spectrometry**; Joshua Silveira; Mark Ridgeway; Jacob Meier; Melvin Park; *Bruker Daltonics, Billerica, MA*
- WP 665 **UPLC Ion Mobility Mass Spectrometry: A New Approach to Authentication and Routine Screening of Ginsenoside Isomers in Functional Food Products**; McCullagh Mike; David Douce; Robert Lewis; *Waters (MS Technologies), Wilmslow, UK*
- WP 666 **Discovery of Pesticide Protomers Using Routine Ion Mobility Screening**; Michael McCullagh¹; Jeff Goshawk¹; Severine Goscinny²; Vincent Hanot²; Kieran Neeson¹; David Eatough¹; Chris Carver¹; ¹*Waters, Manchester, UK*; ²*Institut Scientifique de Santé Publique, Brussels, Belgium*
- WP 667 **Combining an Integrated Microfluidic Device with CCS Ion Mobility Screening for the Analysis of Pesticide Residues in Food**; Michael McCullagh¹; Séverine Goscinny²; Vincent Hanot²; David Douce¹; ¹*Waters (MS Technologies), Wilmslow, UK*; ²*Scientific Institute of Public Health, Brussels, Belgium*
- WP 668 **Using the Routine Separation Dimension and Identification Criteria of UPLC Ion Mobility to Enhance Specificity in Profiling Complex Samples**; Michael McCullagh¹; Kieran J Neeson¹; C. A. M. Pereira²; J. H. Yariwake²; Chris Carver¹; David Douce¹; ¹*Waters Corporation, Manchester, UK*; ²*Universidade de Sao Paulo, Sao Paulo, Brasil*
- WP 669 **Supercharging of Native-Like Proteins and Protein Complexes: Effects of m-Nitrobenzyl Alcohol versus Sulfolane**; Christiane N. Stachl; Samuel J. Allen; Matthew F. Bush; *University of Washington, Seattle, WA*
- WP 670 **Analysis of Motor Oil by Selected Accumulation Ion Mobility Spectrometry**; Kyle Fort¹; William K. Russell¹; Do Yong Kim¹; Desmond Kaplan²; Melvin A. Park³; David H. Russell¹; Mark Ridgeway³; ¹*Texas A&M University, College Station, TX*; ²*Bruker Daltonics, inc., Fremont, CA*; ³*Bruker Daltonics, Inc., Billerica, MA*
- WP 671 **Steroid and Lipid Analysis by High Resolution Ion Mobility-TOF MS**; Michael Groessl¹; Bernhard Dick²; Bruno Vogt²; Richard Knochenmuss¹; ¹*Tofwerk, Thun, Switzerland*; ²*Bern University Hospital, Bern, Switzerland*
- WP 672 **Ion Mobility Spectrometry Tandem Mass Spectrometry (IMS-MSⁿ) and Parallel Dissociation of Plasma Metabolites and Fragments**; Gregory Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- WP 673 **Metabolomics of Plasma Fluids from Apolipoprotein A-V Knockout Mice by Hadamard Transform Ion Mobility Time-of-Flight Mass Spectrometry (HT-IMtofMS)**; Xing Zhang¹; Min Xu²; Patrick Tso²; William Siems¹; Herbert Hill¹;

¹Washington State University, Pullman, WA; ²University of Cincinnati, Cincinnati, OH

- WP 674 **Database to Predict the Collision Cross Section of Glycopeptides by IMS-MS;** Rebecca S. Glaskin¹; Kshiti Khatri¹; Ruwan Kurulugama²; Alex Mordehai²; Joseph Zaia¹; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²Agilent Technologies, Santa Clara, CA
- WP 675 **Ion Mobility-Mass Spectrometry Reveals Significant Structural Rearrangements During the Collision Induced Dissociation of Charge Reduced Protein Complexes;** Russell Bornschein; Shuai Niu; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- WP 676 **A Study of the Effects of Calibrant Choice in Determination of Ion-Neutral Collision Cross Sections via Traveling Wave Ion Mobility;** Rebecca E. Jarratt; Abby S. Gelb; Yuting Huang; Eric D. Dodds; *University of Nebraska-Lincoln, Lincoln, NE*
- WP 677 **An Ion Mobility Spectrometry-Mass Spectrometry Study of Metalated Isomeric Carbohydrates and their Electron Transfer Products;** Yuting Huang¹; Eric D. Dodds²; ¹University of Nebraska-Lincoln, Lincoln, NE; ²University of Nebraska - Lincoln, Lincoln, NE
- WP 678 **Collision Cross Section Dependence upon Glycan Size, Charge State, and Peptide Sequence of High Mannose N-Linked Glycopeptides;** Abby S. Gelb; Yuting Huang; Rebecca E. Jarratt; Eric D. Dodds; *University of Nebraska-Lincoln, Lincoln, NE*
- WP 679 **Ion Mobility-Mass Spectrometry Monitoring of isoxazolidin-5-one Organocatalyzed Synthesis;** Corinne Loutelier-Bourhis; Clisy Maganga; Marie Hubert-Roux; Vincent Levacher; Jean-François Brière; Carlos Afonso; *University of Rouen, Mont Saint Aignan, France*
- WP 680 **Improved Separation Methods for Rapid Analysis of Targeted Small Molecules on IMS/Q-TOF Platform;** Christopher Beekman¹; David L. Wong²; Christian Klein²; Ruwan Kurulugama²; Richard A. Yost¹; ¹University of Florida, Gainesville, FL; ²Agilent Technologies, Santa Clara, CA
- WP 681 **An Artificial Intelligence Technique is used in Optimization of Dual Separation System, IM-QTOF;** Huy Bui; Christian Klein; William Moore; Dung Le; Sandra Tang; William Frazer; Bruce Wang; Gregor Overney; Ruwan Kurulugama; Alex Mordehai; George Stafford; *Agilent Technologies, Santa Clara, CA*
- WP 682 **Structural and Conformational Studies of Non-Covalent Complexes Formed upon Ion Pairing;** Christophe Chendo¹; Momar Touré¹; Olivier Chuzel¹; Stéphane Viel¹; Erik Laurini²; Paola Posocco²; Sabrina Pricl²; Jean-Luc Parrain¹; Laurence Charles¹; ¹Aix-Marseille University, Marseille, France; ²University of Trieste, Trieste, Italy
- WP 683 **Evidence for Unknown Structure Changes in Strained PAH Macrocycles by Fragmentation Ion Mobility Mass Spectrometry;** Wen Zhang; Martin Quernheim; Hans Joachim Räder; Klaus Müllen; *MPI for Polymer Research, Mainz, Germany*
- WP 684 **Discrimination of Large Maltooligosaccharides from Isobaric Dextran and Pullulan using Ion Mobility Mass Spectrometry;** Abdul M Rashid; Gerhard Saalbach; Stephen Bornemann; *John Innes Centre, Norwich, UK*
- WP 685 **Ion Mobility Mass Spectrometry Applied to the Mechanistic Elucidation of Asymmetric Morita-Baylis-Hillman Reaction;** Renan Galaverna; Marla Godoi; Giovana Bataglion; Fernando Coelho; Marcos Eberlin; *State university of campinas, Campinas, Brasil*
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- WP 686 **Experimental Validation of an Analytical Model for Trapped Ion Mobility Spectrometry;** Melvin A. Park¹; Karsten Michelmann²; Joshua Silveira¹; Mark Ridgeway¹; ¹Bruker Daltonics, Inc., Billerica, MA; ²Bruker Daltonik GmbH, Bremen, Germany
- WP 687 **Predictive Mathematical Descriptors of Biological Class Trends in Ion Mobility-Mass Spectrometry Analysis;** Caleb B. Morris; Jody C. May; John A. McLean; *Vanderbilt University, Nashville, TN*
- WP 688 **Technical Advances and Theoretical Performance Assessment of a Spatially Multiplexed Ion Mobility-Mass Spectrometer;** Katrina L. Leaptrot; Jody C. May; John A. Mclean; *Vanderbilt University, Nashville, TN*
- WP 689 **A New Solver to Calculate Ion Density Distribution and Electric Field in Dense Gas;** Roger Giles¹; Vadim Sizykh²; Alina Andreyeva³; ¹Shimadzu Research Laboratory, Manchester, UK; ²Moscow State University of Inst Eng & Informatics, Moscow, Russia; ³(3)Advanced Numerical Simulations, Huddersfield, UK
- WP 690 **Derivation of an Analytical Model for Trapped Ion Mobility Spectrometry;** Karsten Michelmann; Joshua Silveira; Mark Ridgeway; Melvin Park; *Bruker Daltonics, Billerica, MA*
- WP 691 **Theoretical and Experimental Study of Fast Ion Separation and Detection in Liquid;** Yi-Hong Cai; Jia-Der Lin; Yi-Sheng Wang; *GRC, Academia Sinica, Taipei, Taiwan*
- WP 692 **Maximizing the Multiplexing Advantage: Mobility-Specific Sources of Transform Error and Means of Correction;** Brian H. Clowers; Xing Zhang; Zhihau Yu; William F. Siems; *Washington State University, Pullman, WA*
- WP 693 **Accurate Ion Mobility Spectrometer;** Brian Hauck¹; Bill Siems¹; Charles Harden²; Vince McHugh³; Herbert Hill, Jr. ¹; ¹Washington State University, Pullman, WA; ²LEIDOS - US Army ECBC Operations, Gunpowder, MD; ³U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD
- WP 694 **Effects of MALDI Matrix Ions in Traveling Wave Ion Mobility Mass Spectrometry;** Joseph Mwangi; Norman Chiu; *University of North Carolina at Greensboro, Greensboro, NC*
- WP 695 **The Effect of Charge Location in Ion Mobility Mass Spectrometry for Small Molecule Analytes;** Cris Laphorn¹; Frank Pullen¹; Babur Chowdhry¹; George Perkins²; Trevor Dines³; Michael McCullagh⁴; ¹University of Greenwich, Chatham Maritime, UK; ²PerkinElmer Inc, Branford, CT; ³University of Dundee, Dundee, UK; ⁴Waters Corporation, Manchester, UK
- WP 696 **Correlating DMS Simulations with Experiment;** Frank Londry; Brad Schneider; Thomas Covey; *AB SCIEX, Concord, Canada*
- WP 697 **Characterization of Gas Phase Ion/Neutral Interactions in DMS;** David Gode; Dietrich Volmer; *Saarland University, Saarbrücken, Germany*
- WP 698 **Improving Ion Mobility Measurement Sensitivity by Utilizing Helium in an Ion Funnel Trap;** Yehia Ibrahim; Sandilya Garimella; Aleksey Tolmachev; Erin Baker; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 699 **Cytochrome c Conformations Studied by Ion Mobility Spectrometry with Hydrogen-Deuterium Exchange and MS/MS Techniques;** Samaneh Ghassabi Kondalaji; Mahdiar Khakinejad; Stephen Valentine; *Morgantown, WV*

- WP 700 **Conformational Preferences of Peptide – Alkali Metal Ion Adducts: The Effects of Polar Side Chain – Alkali Metal Ion Interactions;** [Chunying Xiao](#); Lisa M. Pérez; David H. Russell; *Texas A&M University, College Station, Texas*
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- WP 701 **Inkjet Printed Gold Nanoparticle Surfaces for the Detection of Biomolecules by Laser Desorption/Ionization Mass Spectrometry;** [Alyssa Marsico](#); Brian Creran; Bradley Duncan; S. Gokhan Elci; Vincent Rotello; Richard Vachet; *University of Massachusetts Amherst, Amherst, Massachusetts*
- WP 702 **Characterization of Monolayer Films of Asymmetric Metallosurfactants by Matrix Assisted Ionization Vacuum Mass Spectrometry;** [Tarick El-Baba](#); Lanka Wickramasinghe; Claudio Verani; Sarah Trimpin; *Wayne State University, Detroit, MI*
- WP 703 **Combined Mass Spectrometric Imaging for Obtaining Site-Specific Information about Nanoparticle Stability in Tissues;** [Sukru Gokhan Elci](#); Bo Yan; Sung Tae Kim; Chang Soo Kim; Krishnendu Saha; Daniel F. Moyano; Vincent M. Rotello; Richard W. Vachet; *University of Massachusetts, Amherst, MA*
- WP 704 **Investigation of Protein Corona on CpG Oligodeoxynucleotides Conjugated Nanotube with Mass Spectrometry;** [Shang Zeng](#); Wenwan Zhong; *University of California, Riverside, Riverside, CA*
- WP 705 **Cluster Ion Source Coupled to a 9.4 T FT-ICR Mass Spectrometer for Experimental Study of Fullerene Formation and Gas-Phase Chemistry;** [Paul W. Dunk](#)¹; Ryan A. Barrett²; Nathan K. Kaiser¹; Alan G. Marshall³; Harold W. Kroto²; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*Florida State University, Tallahassee, FL*; ³*Ion Cyclotron Resonance Prog, Tallahassee, FL*
- WP 706 **Mass Spectrometry-Based Analysis of Graphene Oxide Degradation Products;** [Wentao Jiang](#)¹; Hao Bai¹; Gregg P. Kotchey¹; Wissam A. Saidi¹; Benjamin J. Bythell²; Jacqueline M. Jarvis³; Alan G. Marshall^{2,3}; Rena A.S. Robinson¹; Alexander Star¹; ¹*University of Pittsburgh, Pittsburgh, Pennsylvania*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*; ³*Florida State University, Tallahassee, FL*
- WP 707 **Investigating Engineered Nanomaterial Induced Damage to Genomic DNA via Tandem Mass Spectrometry;** [Elijah J. Petersen](#); Pawel Jaruga; Miral Dizdaroglu; [Bryant C. Nelson](#); *National Institute of Standards and Technology, Gaithersburg, MD*
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- WP 709 **The Secret of Stradivarius: Is it Possible to Clue It?;** [Olga Polyakova](#)¹; Savva Girshenko¹; Slava. Artaev³; Alessandra Tata²; Andreia Porcari²; Eduardo Schmidt²; Marcos Eberlin²; Albert T. Lebedev¹; ¹*Moscow State University, Moscow, Russian Federation*; ²*Thomson Mass Spectrometry Laboratory, Campinas, Brazil*; ³*LECO Corporation, St Joseph, MI*
- WP 710 **Isolation, Structure Elucidation and Reference Synthesis of Impurities in LX1606 by Mass Directed Fraction Collection, MS/MS, TOF/MS and NMR Spectroscopy;** [Leonard O. Hargiss](#); Philip Keyes; Matthew M. Zhao; Weiguo Liu; *Lexicon Pharmaceuticals, Princeton, NJ*
- WP 711 **Comparison of Electrospray Ionization(ESI) and Atmospheric Pressure Chemical Ionization(APCI) of Labile Anti-Malarial Compounds to Monitor Pharmacokinetics of Transdermal Patches;** [Almas Taj Awan](#)¹; Ilza M. O. Sousa²; Fabricio F. Favero²; Nubia C. A. Queiroz²; Marcos N. Eberlin¹; Mary Ann Foglio²; ¹*Thomson Mass spectrometry Laboratory, UNICAMP, Campinas, SP*; ²*CPQBA, UNICAMP, Campinas, SP*
- WP 712 **Characterization of Novel Methylindole-Glutathione-related Conjugates by LC-High Resolution Mass Spectrometry;** [Chenghong Zhang](#); Shuguang Ma; Cornelius Hop; Cyrus Khojasteh; *Genentech, South San Francisco, CA*
- WP 713 **The Use of Linear Ion Trap for HPLC Profiling of Ginsenosides in Plant Extracts and Ginseng Based Products;** [Andrey Stavriani](#); Igor Rodin; Irina Ananieva; Oleg Shpigun; *MSU, Moscow, RU*
- WP 714 **Characterization of Glycosylated Flavonoids in Plant Extracts : A “Same Masses” Nightmare;** [Claude-Paul Lafrance](#); Maxim Maheux; *TransBIOTech, Levis,*
- WP 715 **Proteolytic Activity Elicited during Work-Up Of Human Serum Samples – Obstacle for Biomarker Analysis: Mass Spectrometric Characterization of Cleavage Products;** [Jingzhi Yang](#)¹; Claudia Roewer¹; Cornelia Koy¹; Manuela Russ¹; Martin Sklorz^{2,3}; Ralf Zimmermann^{2,3}; Uwe Fritschen⁴; Juliane C. Finke⁴; Michael O. Glocker¹; ¹*Proteome Center Rostock, University of Rostock, Rostock, Germany*; ²*Institute of Chemistry, University of Rostock, Rostock, Germany*; ³*Helmholtz Zentrum München, Munich, Germany*; ⁴*HELIOS Clinic Emil von Behring, Berlin, Germany*
- WP 716 **Elevated Pressure Improves the Extraction and Identification of Proteins Recovered from Formalin-Fixed, Paraffin-Embedded Tissue Surrogates;** [Carol Fowler](#)¹; Cedric Moore³; Timothy O’Leary²; [Jeffrey Mason](#)¹; ¹*Baltimore VA Medical Center, Baltimore, MD*; ²*Veterans Health Administration, Washington, DC*; ³*Johns Hopkins University, Baltimore, MD*
- WP 717 **LC-MS/MS Impurity Profiling and Quantitation for an Improved Bioprocess for the Production of a Fab Fragment in *E. coli*;** [Anita Krishnan](#); Shirishkumar Patel; Shalvi Shah; Sudheer Babu; Shardul Salunkhe; Sachin Rewanwar; Naidu Mookala; Archana Verma; Nagnath Mandi; Praveen Muneshwar; Sandeep Somani; Ashok Mishra; Brajesh Varshney; Rustom Mody; *Lupin limited, Biotech, Pune, India*
- WP 718 **Discovery and Characterization of a Novel Photo-Oxidative Histidine-Histidine Crosslink in IgG1 Antibody Utilizing ¹⁸O-labeling and Mass Spectrometry;** [Min Liu](#)^{1,2}; Zhongqi Zhang¹; Janet Cheetham¹; Da Ren¹; Zhaohui Sunny Zhou²; [Amgen, Inc.](#), Thousand Oaks, CA; ²*Northeastern University, Boston, MA*
- WP 719 **Comparative Identification Methods of MS Data: Profile Versus Centroid Acquisition and the Advantage of Preliminary Multivariate Curve Resolution (MCR-ALS) Analysis;** [Eva Gorrochategui](#)¹; Yongdong Wang²; Silvia Lacorte¹; Cinta Porte¹; Romà Tauler¹; ¹*Institute of Environ. Assessment & Water Research, Barcelona, Spain*; ²*Cerno Bioscience, Norwalk, VA*
- WP 720 **A New GC “Retention Projection” Database Enables Calculation of Appropriate Retention Time Tolerance Windows without Having Standards Physically on Hand;** [Brian Barnes](#)¹; Michael Wilson²; Peter Carr¹; Mark Vitha³; Corey Broeckling⁴; Adam Heuberger⁴; Jessica Prenni⁴; Gregory Janis⁵; Henry Corcoran⁵; Nicholas Snow⁶; Shilpi Chopra⁶; Ramkumar Dhandapani⁶; Amanda Tawfall⁷; Lloyd Sumner⁷; [Paul Boswell](#)²; ¹*University of Minnesota, Minneapolis, MN*; ²*University of Minnesota, Saint Paul, MN*; ³*Drake University, Des Moines, IA*; ⁴*Colorado State University, Fort Collins, CO*; ⁵*MedTox Laboratories, Saint Paul, MN*; ⁶*Seton Hall University, South Orange, NJ*; ⁷*The Samuel Roberts Noble Foundation, Ardmore, OK*

- WP 721 **Accurate Prediction of Retention in Hydrophilic Interaction Chromatography (HILIC) by Back-Calculation of HPLC Gradient Profiles;** Nu Wang; Paul G. Boswell; *University of Minnesota, Saint Paul, MN*
- WP 722 **Validation of Decoy Models for HRM/SWATH Acquisition as Used in Spectronaut;** Oliver M. Bernhardt; Roland M. Bruderer; Tejas Gandhi; Saša M. Miladinović; Oliver Rinner; Lukas Reiter; *BiognoSYS AG, Zurich, Switzerland*
- WP 723 **Differentiating Gold Nanoparticle Cell Surface Adhesion from Cellular Internalization using Laser Desorption Ionization Mass Spectrometry;** Singyuk Hou; Ying Jiang; Sung Tae Kim; Ziwen Jiang; Vincent Rotello; Richard Vachet; *University of Massachusetts, Amherst, Massachusetts*
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- WP 724 **Isotopic Exchange Mass Spectrometry Reveals Molecular Structure of Natural Organic Matter;** Yury Kostyukevich¹; Alexey Kononikhin¹; Igor Popov²; Eugene Nikolaev¹; ¹*Institute for Energy Problems of Chemical Physics, Moscow, RUSSIA*; ²*IBCP RAS, Moscow, Russian Federation*
- WP 725 **Qual/Quan Discovery Bioanalytical Strategies for Macromolecular Peptides using High Resolution Mass Spectrometry;** Asoka Ranasinghe; Eugene F. Ciccimaro; Celia D'Arienzo; Timothy Olah; *Bristol-Myers Squibb, Princeton, NJ*
- WP 726 **Eliminating Interferences in Serum Extracts using High Resolution Accurate Mass Spectrometry;** Jolaine Hines; Amy Gorsh; Kendall Cradic; Ravinder Singh; Stefan Grebe; *Mayo Clinic, Rochester, MN*
- WP 727 **Characterization of an Improved Ultra-High Resolution Quadrupole Time of Flight (UHR-TOF) Instrument for Proteomics Applications;** Markus Lubeck; Stephanie Kaspar; Annette Michalski; Oliver Raether; Christoph Gebhardt; Carsten Baessmann; *Bruker Daltonik GmbH, Bremen, Germany*
- WP 728 **Utilizing Very High Resolution Fine Isotopic Fragmentation Data to Refine Elemental Composition Determination;** Tim Stratton; *Thermo Fisher Scientific, San Jose, CA*
- WP 729 **High-resolution Two-Dimensional FT-ICR Mass Spectrometry and Applications to Top-Down and Bottom-up Proteomics and Environmental Samples;** Maria van Agthoven¹; Christopher Wootton¹; Andrew Soulby¹; Juan Wei¹; Mark Barrow¹; Lionel Chiron²; Marie-Aude Coutouly²; Marc-André Delsuc³; Christian Rolando⁴; Peter O'Connor¹; ¹*University of Warwick, Coventry, UK*; ²*NMRTEC, Illkirch-Graffenstaden, France*; ³*IGBMC, Illkirch-Graffenstaden, France*; ⁴*Université Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France*
- WP 730 **Faster is Better? A Look at Speed vs Complexity in the Orbitrap Fusion;** Jolene K. Diedrich¹; Antonio F. M. Pinto²; John R. Yates III¹; ¹*The Scripps Research Institute, La Jolla, CA*; ²*CAPES Foundation, Brasilia, Brazil*
- WP 731 **Rapid Accurate Mass Strategy for Photodegradation Study of Machite Green under Natural Sunlight Irritation;** Yanchun Sun¹; Jiehui Hu²; Xiaoyan Xu²; Ting Liu²; Chengyuan Cai²; ¹*Heilongjiang River Fishery Research Institute, Harbin, China*; ²*AB SCIEX, Shanghai, China*
- WP 732 **Utility of High Resolution ESI CID, HCD and ETD MSⁿ for Complete Structural Elucidation of Large Cyclic Peptides and Metabolites;** Eugene F. Ciccimaro¹; Qian Ruan¹; Serhiy Hnatyshyn¹; Timothy Olah¹; Hongxia (Jessica) Wang³; Gary Walker²; Marshall M. Siegel²; ¹*Bristol-Myers Squibb, Princeton, NJ*; ²*MS Mass Spec Consultants, Fair Lawn, NJ*; ³*Thermo Fisher Scientific, San Jose, CA*
- WP 733 **High Resolution Mass Spectrometry (GC-APCI-/LDI-/ESI-FTICRMS) of Heavy Fuel Oil and Particulate Matter Emitted by a Ship Diesel Engine;** Martin Sklorz^{1,2}; Christopher Rüger^{1,2}; Theo Schwemer^{1,2}; Ralf Zimmermann^{1,2}; ¹*University of Rostock, Rostock, Germany*; ²*Helmholtz Zentrum München, Munich, Germany*
- WP 734 **Resolution Requirement for Isotopic Fine Structure Determination of Peptide Fragment with Introduced mDa Stable Isotope Encoding;** Greg T. Blakney¹; Chad Weisbrod¹; Nathan Kaiser¹; Chris L. Hendrickson¹; Alan G. Marshall^{1,2}; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*Dept. of Chemistry, Florida State University, Tallahassee, FL*
- WP 735 **Determination of Site-Specific Protein Disulfide Bond Redox Potentials by Top-Down FT-ICR Mass Spectrometry;** Xiaoyan Guan¹; Nicolas L. Young¹; Alan G. Marshall^{1,2}; ¹*National High Magnetic Field Laboratory, Tallahassee, FL*; ²*Florida State University, Tallahassee, FL*
- WP 736 **Developing an MS-based Platform for High-throughput and Quantitative Assessment of Protein-ligand Interaction: Application in Drug Candidate Screening;** Xin Chen¹; Shanshan Qin¹; Lixin Li²; Cheng Yang²; Wenqing Shui³; ¹*College of Life Sciences, Nankai University, Tianjin, China*; ²*High-throughput Molecular Drug Discovery Center, Tianjin, China*; ³*Tianjin Institute of Industrial Biotechnology, CAS, Tianjin, China*
- WP 737 **Large Scale Targeted Protein Quantification using WISIM-DIA workflow on a Orbitrap Fusion Tribrid Mass Spectrometer;** Reiko Kiyonami¹; Bhavin Patel²; Michael W. Senko¹; Vlad Zabrouskov¹; Jarrett Egerton³; Ying Sonia Ting³; Michael J. Maccoss³; John C. Rogers²; Andreas FR Hühmer¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Rockford, IL*; ³*Univ of Washington, Seattle, WA*
- WP 738 **TMT 10-plex Quantification with Synchronous Precursor selection-MS³ Enables Robust Global Classification of Protein Subcellular Localization in Pluripotent Embryonic Stem Cells;** Andy Christoforou^{1,2}; Claire Mulvey^{1,2}; Lisa M. Breckels¹; Penny Hayward²; Laurent Gatto¹; Rosa Viner³; Alfonso Martinez Arias²; Kathryn S. Lilley¹; ¹*Dept. of Biochemistry, University of Cambridge, Cambridge, UK*; ²*Dept. of Genetics, University of Cambridge, Cambridge, UK*; ³*ThermoFisher Scientific, San Jose, CA*
- WP 739 **Characterization of Metabolites Inmicrosomal Metabolism of aconitineby High-Performance Liquid Chromatography/Quadrupole Ion Trap/Time-Of-Flight Mass Spectrometry;** Cuiping Yang¹; Changkun Li²; Tianhong Zhang¹; Qian Sun²; Yueqi Li²; Guixiang Yang²; Taohong Huang²; Shin-ichi Kawano²; Yuki Hashi²; Zhenqing Zhang¹; ¹*Beijing Institute of Pharmacology and Toxicology, Beijing, China*; ²*Shimadzu (China) Co., Ltd., Shanghai, China*
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- WP 740 **Remote Laser Ablation Electrospray Ionization Mass Spectrometry for Non-Proximate Analysis;** Laine Compton¹; Brent Reschke²; Jordan Friend²; Matthew Powell²; Akos Vertes¹; ¹*George Washington University, Washington, District of Columbia*; ²*Protea Biosciences, Inc., Morgantown, WV*

- WP 741 **Single-probe: A Novel Sampling and Ionization Device for Mass Spectrometry Studies of Single Cells, Biological Tissues, and Protein PTMs;** Zhibo Yang; Ning Pan; Wei Rao; Rachel Vowcicefski; Chuanbin Mao; Xuewei Qu; *University of Oklahoma, Norman, OK*
- WP 742 **A Comparison of Ion Suppression Across Flow Regimes and the Implications of Reduced Suppression on Sensitivity and Assay Precision;** Jay S. Johnson; James Murphy; Paul Rainville; *Waters Corporation, Milford, MA*
- WP 743 **Conical Duct (ConDUCT) ESI Inlet Electrodes Produce Intense Laser-Like Focused Ion Beams with Close to 100% Ion Transmission Efficiency;** Andrew N. Krutchinsky; Julio C. Padovan; Herbert Cohen; Brian T. Chait; *Rockefeller University, New York, NY*
- WP 744 **Comprehensive Mass Spectrometric Analysis of Ablated Proteins in Ultrafast Desorption by Vibrational Excitation (DIVE);** Marcel Kwiatkowski¹; Marcus Wurlitzer¹; Ling Ren²; Yinfei Lu²; Wesley Robertson²; R.J. Dwayne Miller²; Hartmut Schlüter¹; ¹*University Medical Centre Hamburg-Eppendorf, Hamburg, Germany*; ²*MPSD for Structural Dynamics, Hamburg, Germany*
- WP 745 **Sub-ambient Pressure Ionization Nanoelectrospray (SPIN): High Sensitivity Detection and Extended Structural Characterization of Labile Compounds Unattainable by Conventional ESI;** Jonathan T. Cox; Scott R. Kronewitter; Anil Shukla; Ronald J. Moore; Keqi Tang; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 746 **Novel Quantitative Strategies for Condensed Phase Membrane Introduction Mass Spectrometry: Mitigating Ion Suppression and Extending Linear Dynamic Range;** Kyle D. Duncan^{1,2}; Gregory W. Vandergriff¹; Mathias Baltes¹; Erik T. Krogh^{1,2}; Christopher G. Gill^{1,2}; ¹*Applied Environmental Research Laboratories (AERL), Vancouver Island University, Nanaimo, Canada*; ²*Chem. Dept, University of Victoria, Victoria, BC, Canada*
- WP 747 **Slug Flow Microextraction NanoESI with Real-Time Derivatization for Rapid Analysis of Biofluid Samples;** Yue Ren; Morgan McLuckey; Jiangjiang Liu; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- WP 748 **Persistent Multiply Charged Ion Signals Generated by Liquid MALDI Enables Sensitive ETD and Ion Mobility MS Analysis;** Jeff Brown^{1,2}; Michael Morris²; Pavel Ryumin¹; Rainer Cramer¹; ¹*University of Reading, Reading, UK*; ²*Waters Corporation, Wilmslow, UK*
- WP 749 **Controlling Ionization Chemistry in Plasma-Assisted Reaction Chemical Ionization;** Haopeng Wang¹; Ninghang Lin¹; Kaveh Kahen²; Hamid Badiei²; Kaveh Jorabchi¹; ¹*Georgetown University, Washington, DC*; ²*PerkinElmer Inc., Woodbridge, Canada*
- WP 750 **Optimization of Thin Film Solid Phase Microextraction (SPME) Devices for Direct Analysis in Real Time (DART) Coupled with Tandem MS;** Germán Augusto Gómez-Ríos; Nathaly Reyes-Garcés; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- WP 751 **Characterising Linear and Radial Surface Acoustic Wave Nebulisation Devices for Optimising Protein Ionisation by Design;** Andrew Dennison¹; Yifan Li¹; Scott Heron²; C. Logan Mackay¹; David Goodlet²; Patrick Langridge-Smith¹; Anthony Walton¹; Andrew Mount¹; ¹*The University of Edinburgh, Edinburgh, UK*; ²*University of Maryland, Baltimore, MD*
- WP 752 **Signal and Signal-to-noise Enhancement Mediated by Helium with Coanda Effect Electrospray Ionization (CEESI) Source;** Yixin Zhu²; Tingting Lv²; Peiming Song²; Rong Wang¹; ¹*Icahn School of Medicine at Mount Sinai, New York, NY*; ²*Zhejiang Haochuang, Hangzhou, China*
- WP 753 **Development of a Vacuum Ultraviolet Photoionization Source for Gas Chromatography used with a High Resolution Time of Flight Mass Spectrometer;** Lloyd Allen; Roza Wojcik; Viatcheslav Artaev; *LECO Corp., Saint Joseph, MI*
- WP 754 **Development of a Chip-Based Nanobore Column Platform with Universal Connectivity, Column Heating and Sheath Gas Capability;** Helena Svobodova¹; Peter Wang²; Amanda Berg¹; Gary A. Valaskovic¹; ¹*New Objective, Inc., Woburn, MA*; ²*New Objective, Inc., Shanghai, China*
- WP 755 **Matrix Assisted Ionization Vacuum (MAIV) Using FT-ICR;** Evgenia Tisdale¹; Beixi Wang²; Sarah Trimpin²; Charles L. Wilkins¹; ¹*University of Arkansas, Fayetteville, AR*; ²*Wayne State University, Detroit, MI*
- WP 756 **Flow Dynamics Technique for Sampling and Separation of Neutrals from Analytes Based on Their Axial Momentum Density Differences;** Gary Salazar^{1,2}; Soenke Szidat^{1,2}; ¹*Depart. of Chem. and Biochem., Univ. of Bern, Bern, Switzerland*; ²*Oeschger Centre for Climate Change Research, Bern, Switzerland*
- WP 757 **Development of a Novel TRESI-MS Capillary Mixing Device and Proof of Concept via Characterization of Known Protein Interactions;** Nicholas Zinck¹; Ann-Katherine Stark Stark¹; Michal Sharon²; Derek Wilson¹; ¹*York University, Toronto, Canada*; ²*Weizmann Institute of Science, Rehovot, Israel*
- WP 758 **Further Developments Interfacing a High Performance Ion Mobility Spectrometer to LTQ Series Mass Spectrometers;** Robert Jackson; Adam Graichen; Mark Osgood; Ching Wu; *Excellims Corporation, Acton, MA*
- WP 759 **Development of an Inline Microfluidic Electrochemical Cell to Study Carbon Dioxide Reduction Mechanisms;** Luke Wooster; Yeon Jae Ko; Alessandra Ferzoco; *Rowland Institute at Harvard, Cambridge, MA*

FAIMS and DMS, 760 - 779

- WP 760 **Optimization and Performance Characterization of a Microscale FAIMS Chip Coupled to an Orbitrap Mass Spectrometer;** Lauren Brown¹; Robert Smith¹; Alastair Taylor¹; Michael Winter¹; Danielle Toutoungi¹; Dirk Nolting²; Alexander Makarov²; ¹*Owlstone Ltd, Cambridge, UK*; ²*ThermoFisher Scientific, Bremen, Germany*
- WP 761 **On a Novel Interface for Electrospray Ionization (ESI)-Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) and Significant Improvement in Sensitivity;** Satendra Prasad; Michael W. Belford; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- WP 762 **Effect of Electrode Geometry on FAIMS Gas Flow Focusing and Lateral Diffusion;** Jean-Jacques Dunyach; Satendra Prasad; Michael Belford; *Thermo Fisher Scientific, San Jose, CA*
- WP 763 **Effect of FAIMS Gas Velocity on Resolution, Sensitivity, and Nanospray Formation;** Michael Belford; Satendra Prasad; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- WP 764 **Development and Application of FAIMS for the Investigation of FGF Signaling;** Hongyan Zhao; Debbie L. Cunningham; Andrew J. Creese; John K. Heath; Helen J. Cooper; *School of Biosciences, University of Birmingham, Birmingham, UK*
- WP 765 **FAIMS Coupled with HCD Product Ion-Triggered ETD Mass Spectrometry for the Analysis of N-glycosylation in Proteins;** Gloria N. Ulasi; Andrew Creese; Cleidiane G. Zampronio; Helen J. Cooper; *School of Biosciences, University of Birmingham, Egbaston, UK*



- WP 766 **FAIMS Fractionation Improves Protein Identification for Low-Abundance Samples;** Kristian E. Swearingen; Jason M. Winget; Michael R. Hoopmann; Robert L. Moritz; *Institute for Systems Biology, Seattle, WA*
- WP 767 **Differential Ion Mobility Separations in Pure Helium and He Mixtures using Microchips;** Alexandre A. Shvartsburg; Yehia Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 768 **Determination of Solvent Effects from Ionization Source on Differential Ion Mobility Spectrometry Separations;** Brandon Santiago; Gary Glish; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- WP 769 **Differential Mobility Separation Pre-filtration on a Portable, Compact Mass Spectrometer;** Spiros Manolakos; Theresa Evans-Nguyen; Francy Sinatra; James Alberti; *The Charles Stark Draper Laboratory, Tampa, FL*
- WP 770 **Linked Scanning of Helium and Compensation Voltage to Improve the Resolving Power of Differential Ion Mobility Spectrometry Separations;** Rachel Harris; Samantha Isenberg; Brandon Santiago; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- WP 771 **Improved DMS Performance with a Jet Injector Inlet;** Brad Schneider¹; Erkinjon Nazarov²; Thomas Covey¹; ¹AB SCIEX, Concord, Canada; ²Draper Laboratories Bioengineering Center, Tampa, FL
- WP 772 **Improved Mass Spectrometer Robustness with DMS Pre-Filtering;** Yang Kang; Bradly Schneider; Thomas R. Covey; *AB Sciex, Concord, Canada*
- WP 773 **Discovery of Abundant, Ubiquitous and Intriguing Contaminants in Drinking Water using Differential Ion Mobility and Soft Mass Spectrometry;** Wojciech Gabryelski¹; Jadwiga Lyczko¹; Daniel Beach²; ¹University of Guelph, Guelph, Canada; ²National Research Council Canada, Halifax, Canada
- WP 774 **Feasibility Study on the Detection of Volatile Organic Compounds (VOCs) from Potato Tuber Soft Rot by Differential Mobility Spectrometry (DMS);** Lav R. Khot¹; Jessica Tufariello²; Ashley Almaguer¹; Eric J. Lynch³; Paul J. Rauch³; Dennis A. Johnson⁴; Nora Olsen⁵; William Siems²; Herbert H. Hill²; ¹Biological Systems Engineering WSU, Pullman, WA; ²Chemistry WSU, Pullman, WA; ³Chemring Sensors and Electronic Systems, Charlotte, NC; ⁴Plant Pathology WSU, Pullman, WA; ⁵Plant, Soil, and Entomological Sciences UI, Moscow, ID
- WP 775 **Rapid Identification of β -carboline Hallucinogens: Harmine and Harmaline, by Pressure Cycling Technology (PCT) and DMS-MS;** Adam B. Hall¹; Amol Kafle¹; Alex Thompson³; Frederick Li²; Kaitlyn Duffy¹; James Glick¹; Stephen L. Coy¹; Paul Vouros¹; ¹Northeastern University, Boston, MA; ²Boston University School of Medicine, Boston, MA; ³Vermont Forensic Laboratory, Waterbury, VT
- WP 776 **Targeted Analysis of Polar Analytes by DMS-MS for Radiation Biodosimetry;** Amol Kafle¹; Stephen Coy¹; Fred Li¹; Evagelia Laiakis²; Albert Fornace²; Paul Vouros¹; ¹Northeastern University, Boston, MA; ²Georgetown University, Washington, DC
- WP 777 **The Application of Differential Mobility Spectrometry(DMS) to the Characterization of the Lipid Profile of Commercially Available Olive Oils;** Paul C. Winkler¹; Paul Baker²; Christopher Borton¹; ¹AB Sciex, Golden, CO; ²AB Sciex, Framingham, MA
- WP 778 **Trimethylation and Chemical Modifiers in IMS/MS Peptide Analysis: Performance Enhancement Through Solution- And Gas-Phase Chemistry;** Voislav Blagojevic; Amanda De Filippis; Diethard K. Bohme; *York University, Toronto, Canada*
- WP 779 **Conformer Isolation in Intrinsically Disordered Protein Ensembles using DMS-MS;** Shaolong Zhu¹; Larry Campbell²; Yves LeBlanc²; Derek J. Wilson¹; ¹York University, Toronto, Canada; ²AB SCIEX, Toronto, Canada



7:30 - 8:00 am Set up all Thursday posters
 10:30 am - 1:00 pm Odd-numbered posters present
 12:00 - 2:30 pm Even-numbered posters present
 2:30 - 3:00 pm Remove all Thursday posters

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Informatics: Systems Biology.....	041-046
Informatics: Crosslinking and Structure Analysis.....	048-056
Informatics: Intact Proteins.....	057-064
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Imaging MS: Instrumentation, 001 - 012

- ThP 001 **Optimization of the MALDI Imaging Laser Repetition Rates using an Orthogonal MALDI Mass Spectrometer;** Emmanuelle Claude; Mark Towers; James Langridge; *Waters corporation, Manchester, UK*
- ThP 002 **Modifications to a Linear Time-of-Flight Mass Spectrometer for Mass Resolved Microscopy with the PimMS Camera;** Edward Halford¹; Benjamin Winter¹; Simon King¹; Mark Mills²; Steve Thompson²; Vic Parr²; Jaya John John¹; Andrei Nomerotski³; Claire Vallance¹; Renato Turchetta⁴; Mark Brouard¹; ¹*University of Oxford, Oxford, UK*; ²*SAI Ltd., Manchester, UK*; ³*Brookhaven National Laboratory, Upton, NY*; ⁴*Rutherford Appleton Laboratory, Oxford, UK*
- ThP 003 **Toward Subcellular MALDI-MS Imaging of Plant Tissues by Modification of MALDI-LTQ-Orbitrap Optics;** Andrew Korte^{1,2}; Young Jin Lee^{1,2}; ¹*Iowa State University, Ames, IA*; ²*Ames Laboratory - US DoE, Ames, IA*
- ThP 004 **Vertically Aligned Transmission Geometry Laser Ablation into a Non-Contact Liquid Vortex Capture Probe for Mass Spectrometry Imaging;** Gary J. Van Berkel; Olga Ovchinnikova; Deepak Bhandari; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 005 **Multimodal Chemical and Physical Surface Characterization on a Combined AFM-MS Platform;** Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 006 **Comparison of UV-MALDI and IR-MALDESI Mass Spectrometry Imaging of Biological Tissue Sections;** Milad Nazari¹; Elias Rosen¹; Mark T. Bokhart¹; Corbin Thompson²; Craig Sykes²; Angela D. M. Kashuba²; David C. Muddiman¹; ¹*North Carolina State University, Raleigh, NC*; ²*The University of North Carolina, Chapel Hill, NC*
- ThP 007 **Toward High Spectral and Spatial Resolution Mass Spectrometry Imaging of Biological Tissue Sections by IR-MALDESI Coupled to the Q Exactive;** Eli Rosen; Guillaume Robichaud; Jeremy Barry; David C. Muddiman; *NC State University, Raleigh, NC*

- ThP 008 **Multiple MS/MS Transition Monitoring in a Single Laser Shot on a MALDI TOF/TOF Mass Spectrometer;** Boone Prentice; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- ThP 009 **Tissue Protein Imaging at 2.5µm Spatial Resolution and High Speed using Transmission Geometry MALDI Source Integrated into a TOFMS Instrument;** Andre Zavalin¹; Junhai Yang¹; Kevin Hayden²; Marvin Vestal²; Richard Caprioli¹; ¹*Vanderbilt University, Nashville, TN*; ²*SimulTOF Systems, Sudbury, MA*
- ThP 010 **Mass Spectrometry Imaging of Biological Systems using Laser Ablation Plume Capture in Aerosol (LAPCA);** Jonathan Brauer; Jan Sunner; Iwona Beech; Eric Kaufman; *University of Oklahoma, Norman, OK*
- ThP 011 **Improved Biological Imaging with Gas Cluster Ion Beams;** John Fletcher¹; Tina Angerer¹; Paul Blenkinsopp²; Andrew Ewing^{1,3}; ¹*University of Gothenburg, Gothenburg, Sweden*; ²*Ionoptika Ltd, Southampton, UK*; ³*Chalmers University of Technology, Gothenburg, Sweden*
- ThP 012 **Development of New Stigmatic Imaging Mass Spectrometer and its Application to surface Analysis of High Functional Organic Materials;** Jun Aoki; Hisanao Hazama; Kunio Awazu; Michisato Toyoda; *Osaka University, Toyonaka-Shi, Japan*
- Informatics: Quantitation/Validation, 013 - 036**
- ThP 013 **A Novel and Straightforward Experimental Null Strategy Enables Accurate Evaluation and Control of False-Discovery of Significantly-Altered-Proteins in Label-Free Quantitative Proteomics;** Xiaomeng Shen; Jun Qu; Jun Li; *University at Buffalo, Buffalo, New York*
- ThP 014 **Systematic Assessment of Survey Scan- and MS2-Based Strategies for Label-Free Quantitative Proteomics using High-Resolution MS Data;** Chengjian Tu¹; Jun Li¹; Qianhu Sheng²; Ming Zhang¹; Jun Qu¹; ¹*University at Buffalo, Buffalo, NY*; ²*Vanderbilt University, Nashville, TN*

- ThP 015 **Comparison of High-End Software for label Free Quantitative Proteomics**; Alon Savidor¹; Stefan Tenzer²; Joerg Kuharev²; Yishai Levin¹; ¹Weizmann Institute of Science, Rehovot, Israel; ²University Medical Center of the Johannes Gutenbe, Mainz, Germany
- ThP 016 **Comparison of Label Free Quantification Tools**; Lei Xin¹; Baozhen Shan¹; Hao Lin¹; Weiwu Chen¹; Mohammad Rahman¹; Bin Ma²; ¹Bioinformatics Solutions Inc., Waterloo, CANADA; ²University of Waterloo, Waterloo, ON
- ThP 017 **Protein Identification and Quantitative Analysis with N-Terminal Sequencing by Mass Spectrometry**; Baozhen Shan; Hao Lin; *Bioinformatics Solutions Inc., Waterloo, Canada*
- ThP 018 **False Quantification in SILAC Proteomic Experiments**; Chris McKennan; Hua Ding; Lynn Spruce; Steven H. Seeholzer; *Children's Hospital of Philadelphia, Philadelphia, PA*
- ThP 019 **Systematic Comparison of Super-SILAC and Label-Free Quantification for Single-Shot Proteome Analysis**; Andreas Tebbe; Martin Klammer; Stefanie Sighart; Christoph Schaab; Felix Oppermann; Henrik Daub; *Evotec München, Munich, Germany*
- ThP 020 **Estimating Effects of Peptide Co-Fragmentation on iTRAQ Quantification by Simulating Multiplexed Spectra for Reliable Identification of Differentially Expressed Peptides**; Honglan Li¹; Kyu-Baek Hwang¹; Dong-Gi Mun²; Hokeun Kim²; Hangeore Lee²; Sang-Won Lee²; Eunok Paek³; ¹Soongsil University, Seoul, Republic of Korea; ²Korea University, Seoul, Republic of Korea; ³Hanyang University, Seoul, Republic of Korea
- ThP 021 **Census 2: Isobaric Labeling Data Analysis in an Automated Way**; Robin Park; Aaron Aslanian; Daniel B. McClatchy; Harshil Shah; Xuemei Han; John Yates; *The Scripps Research Institute, San Diego, CA*
- ThP 022 **Logical Bayesian Networks for Proteomics**; Kurt De Grave; Jan Ramon; *KU Leuven, Leuven, Belgium*
- ThP 023 **Statistical Analysis of Bayesian Hierarchical Inversion for MRM Protein Quantification and QDA Serum Sample Classification**; Laurent Gerfault¹; Amna Klich²; Catherine Mercier²; Pascal Roy²; Jean François Giovannelli³; Audrey Giremus³; Pierre Mahe⁴; Jean Philippe Charrier⁵; Bruno Lacroix⁵; Pierre Grangeat¹; ¹CEA, Leti, Minatec Campus, Grenoble, France; ²HCL, Univ. Lyon 1, CNRS UMR 5558, Lyon, France; ³Univ. Bordeaux, IMS, UMR 5218, Bordeaux, France; ⁴bioMérieux, Grenoble, France; ⁵bioMérieux, Marcy L'etoile, France
- ThP 024 **Identification and Verification of the Missing Proteins for the C-HPP by Using the Mass Spectral Library and MRM Technique**; Jin-Young Cho; Hyoung-Joo Lee; Seul-Ki Jeong; Kwang-Youl Kim; Young-Ki Paik; *YPRC, Seoul, Korea, Republic*
- ThP 025 **CPTAC Assay Portal: a community Web-Based Repository for Well-Characterized Quantitative Targeted Proteomics Assays**; Jeff Whiteaker¹; Goran Halusa²; Andrew Hoofnagle³; Vagisha Sharma³; Brendan MacLean³; Ping Yan¹; John Wrobel⁴; Jacob Kennedy¹; DR Mani⁵; Lisa Zimmerman⁶; Matthew Meyer⁷; Mehdi Mesri⁸; Henry Rodriguez⁸; Amanda Paulovich¹; ¹Fred Hutchinson Cancer Research Center, Seattle, WA; ²Leidos Biomedical Research Inc, Frederick, MD; ³University of Washington, Seattle, WA; ⁴University of North Carolina, Chapel Hill, NC; ⁵Broad Institute, Cambridge, MA; ⁶Vanderbilt University School of Medicine, Nashville, TN; ⁷Washington University School of Medicine, St. Louis, MO; ⁸National Cancer Institute, Bethesda, MD
- ThP 026 **A Scientific Workflow for Automatic Peptide Selection for Targeted Proteomics Experiments**; Yassene Mohammed^{1,2}; Dominik Domanski³; Angela Jackson¹; Derek Smith¹; Andre Deelder²; Magnus Palmblad²; Christoph Borchers^{1,4}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²Center for Proteomics and Metabolomics, Leiden Univ, Leiden, The Netherlands; ³Polish Academy of Sciences, Warsaw, Poland; ⁴UVI Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 027 **Protein Prospector as a Component in a Label Free/ SRM Pipeline**; Peter R Baker¹; Anatoly Urisman²; Robert Chalkley²; ¹UCSF, Rokitnica, POLAND; ²UCSF, San Francisco, CA
- ThP 028 **MS-Umpire: Java Open-Source MS¹ Quantitation Software Based on Untargeted Feature Detection Algorithm for Proteomics and Metabolomics Data**; Chih-Chiang Tsou; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- ThP 029 **Unprecedented Quantitative Evaluation of LC-MS Isotope Trace Feature Detection Using Ground Truth Data**; Rob Smith; Ryan Money; John Prince; Dan Ventura; *Brigham Young University, Provo, UT*
- ThP 030 **Novel Proteomics Mass Spectrometry Simulation in Java: JAMSS**; Rob Smith; John Prince; *Brigham Young University, Provo, UT*
- ThP 031 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data**; Luis Mendoza¹; David D. Shteynberg¹; Joseph Slagel¹; Michael R. Hoopmann¹; Henry Lam²; Jimmy Eng³; 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 032 **A GPU-Powered, Massively Parallel Nonparametric Statistics Server for Analysis and Exploration of Large-Scale Quantitative Data between and across Quantitative Experiments**; John P. Wilson¹; Eric Paniagua¹; Robert M. Farber²; Darryl J.C. Pappin¹; ¹Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; ²Blackdog Endeavors LLC, Gig Harbor, WA
- ThP 033 **PeptideDepot Plugin: Using Statistical Tool to Improve Quality of Quantitative Proteomics Data Generated by Mass Spectrometry**; Qinqin Ji¹; Samantha Beik²; Arthur Salomon^{1,2}; ¹Department of Chemistry, Brown University, Providence, RI; ²Department of Molecular Biology, Cell Biology, and, Providence, RI
- ThP 034 **ProteoSuite v1.0 – An Open Source Framework for Quantitative Proteomics Analysis Based on PSI Data Standards**; Faviel Gonzalez¹; Andrew Collins¹; Jun Fan²; Huaizhong Zhang³; Andrew Dowsey³; Henning Hermjakob⁴; Conrad Bessant²; Simon Hubbard³; Andrew Jones¹; ¹University of Liverpool, Liverpool, UK; ²Queen Mary University of London, London, UK; ³University of Manchester, Manchester, UK; ⁴European Bioinformatics Institute, Cambridge, UK
- ThP 035 **Multi-Instrument, Skyline-Based Comparison of DIA Peptide Identification and Statistical Confidence Tools Enables Improved, Novel Peak Scoring Strategy**; Dario Amodè¹; Don Marsh²; Hannes Rost³; Lucia Espona Pernas³; George Rosenberger³; Ruedi Aebersold³; Parag Mallick¹; Michael J. Maccoss²; Brendan Maclean²; ¹Stanford University, Palo Alto, California; ²Univ of Washington, Seattle, WA; ³ETH Zurich, Zurich, Switzerland
- ThP 036 **Evaluation of Progenesis QI for Proteomics and Progenesis Post-Processor (PPP) as a Simplified Workflow for Ion-Mobility Enabled Data-Independent SILAC Studies**; Joanne B. Connolly¹; Lee A Gettings¹; Kelly McMahon¹; Robert Tonge¹; Johannes Pc Vissers¹;

Anthony D Whetton²; Andrew R Jones³; James Langridge¹;
¹Waters Corporation, Manchester, UK; ²University of
Manchester, Manchester, UK; ³University of Liverpool,
Liverpool, UK

Informatics: Pathway Analysis, 037 - 040

ThP 037 **Improved Peak Detection and Deconvolution of Native Protein Complex Electrospray Mass Spectra**; Jonathan Lu; Michael Trnka; Shenheng Guan; Alma Burlingame; University of California, San Francisco, San Francisco, CA

ThP 038 **Quantitative Proteomics to Unravel the Expression and Translocation of MET Proto-Oncoprotein to Mitochondria**; Kae Hwan Sim; Siu Kwan SZE; School of Biological Sciences, Nanyang Technological University, Singapore 637551, SINGAPORE

ThP 039 **Using Causal Discovery Techniques to Infer Signaling Pathways from Mass Spectrometry Data**; Jennifer Teubl¹; Kelly Ruggles¹; Himanshu Grover¹; Philipp Mertins²; Karl Clauser²; Sherri R. Davies³; R. Reid Townsend³; Matthew J. Ellis³; Steven A. Carr²; David Fenyo¹; ¹NYU Langone Medical Ctr, Ny, NY; ²Broad Institute, Cambridge, MA; ³Washington University, St. Louis, MO

ThP 040 **Pathway Enrichment Analysis for Multi-omic Data using netSVM**; Li Chen; Yuan Tian; Caitlin Choi; Shisheng Sun; Jianying Zhou; Hui Zhang; Daniel Chan; Zhen Zhang; Johns Hopkins School of Medicine, Baltimore, MD

Informatics: Systems Biology, 041 - 046

ThP 041 **A Novel Method for Integration of Proteomic and Transcriptomic Data**; Ekaterina Mostovenko¹; Cheryl Lichti¹; Qianghu Wang²; Erik Sulman²; Carol Nilsson¹; ¹UTMB Galveston, Galveston, TX; ²University of Texas M.D. Anderson Cancer Center, Houston, TX

ThP 042 **Co-Expression Network Analysis of Quantitative Proteomics Data: A New Approach for Studying Neuropsychiatric Disease**; Matthew L MacDonald¹; Ying Ding²; Jason Newman¹; David A Lewis¹; Robert A Sweet¹; Nathan Yates²; ¹University of Pittsburgh, Dept of Psychiatry, Pittsburgh, Pennsylvania; ²University of Pittsburgh, Biomedical Mass Spectr, Pittsburgh, Pennsylvania

ThP 043 **Construction and Assessment of Individualized Proteogenomic Databases for Large-Scale Analysis of Non-Synonymous Single Nucleotide Variants**; Karsten Krug; Sasa Popic; Alejandro Carpy; Katarina Matic; Christoph Taumer; Boris Macek; Proteome Center Tuebingen, University of Tuebingen, Tuebingen, Germany

ThP 044 **Flexible, Accessible and Reproducible Workflows for Tandem Proteogenomic and Metaproteomic Analysis using the Galaxy-P Platform**; Pratik Jagtap¹; Julie Yang²; Getiria Onsongo⁴; Joel Kooren²; Sricharan Bandhakavi³; James Johnson⁴; Joel Rudney²; Tim Griffin²; ¹Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN; ²University of Minnesota, Minneapolis, MN; ³Bio-Rad Laboratories, Hercules, CA; ⁴Minnesota Supercomputing Institute, Minneapolis, MN

ThP 045 **Proteogenomics as a Crucial Tool in the Search for Short Secreted Proteins**; Ira Cooke^{1,2}; Dan Jones^{3,4}; Cecilia Deng⁵; Pierre Faou¹; Nathan Hall²; Vignesh Jayachandran¹; Michael Liem¹; Adam Taranto³; Kim Plummer³; Suresh Mathivanan¹; ¹Department of Biochemistry, La Trobe University, Melbourne, Australia; ²Life Sciences Computation Centre (VLSCI), Melbourne, Australia; ³Department of Botany, La Trobe University, Melbourne, Australia; ⁴Plant Biosecurity CRC, Canberra, Australia; ⁵Institute for Plant and Food Research, Auckland, New Zealand

ThP 046 **Mass Spectrometry based Draft of the Human Proteome**; Mathias Wilhelm¹; Judith Schlegel²; Hannes Hahne¹; Amin Moghaddas Gholami¹; Marcus Lieberenz²; Emanuel Ziegler²; Lars Butzmann²; Siegfried Gessulat²; Harald Marx¹; Mikhail Savitski³; Karsten Schnatbaum⁴; Ulf Reimer⁴; Holger Wenschuh⁴; Marcus Bantscheff³; Anja Gerstmair²; Franz Faerber²; Bernhard Kuster¹; ¹Technical University Munich, Freising, Germany; ²SAP AG, Walldorf, DE; ³Cellzome, Heidelberg, DE; ⁴JPT Peptide Technologies, Berlin, DE

Informatics: Crosslinking and Structure Analysis, 048 - 056

ThP 048 **Identifying Cross-linked Peptides using Protein Prospector**; Robert Chalkley¹; Michael Trnka¹; Nicholas Michael²; Peter R Baker¹; ¹UCSF, San Francisco, CA; ²Reading Scientific Services Ltd, Reading, UK

ThP 049 **Comprehensive Identification of Disulfide Bonds Using Proteinase K Digestion and Second-Order Crosslinking Analysis**; Karl Makepeace¹; Jason Serpa¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada

ThP 050 **Application of a Fast Sorting Algorithm to the Assignment of Mass Spectrometric Crosslinking Data**; Evgeniy Petrotchenko¹; Carol Parker¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada

ThP 051 **Optimizing pLink for Disulfide-bond Analysis**; Sheng-Bo Fan¹; Shan Lu²; Bing Yang²; Jia-Ming Meng¹; Chi Hao¹; Long Wu¹; Kun Zhang¹; Rui-Xiang Sun¹; Meng-Qiu Dong²; Si-Min He¹; ¹ICT, Chinese Academy of Sciences, Beijing, China; ²National Institute of Biological Sciences, Beijing, China

ThP 052 **Software Tools for Improved Efficiency and Automated Interpretation of Mass Spectrometric Analysis of Chemically Crosslinked Proteins**; Guanghui Wang¹; Kevin Ramkissoon²; Jenna Dumond²; Joan Ferraris²; Maurice Burg²; Marjan Gucek¹; ¹Proteomics Core, NHLBI, NIH, Bethesda, MD; ²LKEM, NHLBI, NIH, Bethesda, MD

ThP 053 **Application of Non-selective Photoreactive Cross-linking in Mass Spectrometry-based Structural Proteomics**; Kuan-Chieh Peng; Pang-Hung Hsu; National Taiwan Ocean University, Keelung, Taiwan

ThP 054 **Analysis of Protein-Protein Interactions using Chemical Cross-Linking Mass Spectrometry (CXMS): Novel Computational Approaches**; Mihir Jaiswal^{1,2}; Nathaniel Crabtree^{1,2}; Michael Bauer²; Roger Hall²; Kevin Raney²; Boris Zybailov^{1,2}; ¹University of Arkansas at Little Rock, Little Rock, AR; ²University of Arkansas for Medical Sciences, Little Rock, AR

ThP 055 **Metaproteomic Protein Identification Based on a Species-Level Similarity Correction**; Anke Penzlin; Martin Lindner; Joerg Doellinger; Wojtek Dabrowski; Andreas Nitsche; Bernhard Renard; Robert Koch Institute, Berlin, Germany

ThP 056 **¹⁴N/¹⁵N DXMSMS Match Program for the Automated Analysis of LC/ESI-MS/MS Crosslinking Data from Experiments Using ¹⁵N Metabolically Labeled Proteins**; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada

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ThP 057 **Automated Protein Identification and Sequencing Using Top-Down MS Data**; Christian Heckendorf; Roger Theberge; Jean Spencer; Catherine E. Costello; Mark E. Mccomb; *Boston University School of Medicine, Boston, MA*

ThP 058 **ProSight Lite: Freeware for Targeted Top Down Protein Mass Spectrometry and PTM Localization**; Ryan Fellers¹; Richard Leduc²; Xiang Yu¹; Bryan Early¹; Paul Thomas¹; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Indiana University, Bloomington, IN*

ThP 059 **Improvements upon the C-Score: a Bayesian Framework for Proteoform Characterization in Top Down Proteomics**; Paul Thomas¹; Ryan Fellers¹; Bryan Early¹; Joseph Greer¹; Richard Leduc²; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Indiana University, Bloomington, IN*

ThP 060 **A Framework for Error-Tolerant Identification and Characterization of Protein Complexes by Database Searching and Top Down Tandem Mass Spectrometry**; Pierre C. Havugimana; Owen S. Skinner; Philip D. Compton; Bryan P. Early; Joseph B. Greer; Ryan T. Fellers; Neil L. Kelleher; *Northwestern University, Evanston, IL*

ThP 061 **Differential Profiling of Intact Proteins Using a Novel Two-Pass Approach**; Norton Kitagawa; Christine Miller; Steven M. Fischer; Yinghang Yang; Stephen Madden; *Agilent Technologies, Inc., Santa Clara, CA*

ThP 062 **A Top-Down Driven Approach To De Novo Protein Sequencing**; Kira Vyatkina¹; Lennard Dekker²; Si Wu³; Vitalii Demyanyuk⁴; Xiaowen Liu⁵; Mikhail Dvorkin¹; Sonya Alexandrova¹; Martijn M. Vanduijn²; Theo M. Luider²; Nikola Tolic³; Ljiljana Pasa-Tolic³; Pavel A. Pevzner^{1,6}; ¹*SPb Academic University, St Petersburg, Russian Federation*; ²*Erasmus Medical Center, Rotterdam, Netherlands*; ³*PNNL, Richland, WA*; ⁴*SPb National Research University IFMO, St Petersburg, Russian Federation*; ⁵*IUPUI, Indianapolis, IN*; ⁶*UCSD, La Jolla, CA*

ThP 063 **Complete and Confident Protein Characterization Using Top-down Mass Spectrometry and Isotopic Envelope Fingerprinting**; Zhixin Tian; kaijie Xiao; *Department of Chemistry, Tongji University, Shanghai, China*

ThP 064 **De novo protein sequencing by combining top-down and bottom-up tandem mass spectra**; Xiaowen Liu¹; Lennard Dekker²; Si Wu³; Martijn Vanduijn²; Theo Luider²; Nikola Tolic³; Mikhail Dvorkin⁴; Sonya Alexandrova⁴; Kira Vyatkina⁴; Ljiljana Pasa-Tolic³; Pavel Pevzner⁵; ¹*IUPUI, Indianapolis, IN*; ²*Erasmus Medical Center, Rotterdam, Netherlands*; ³*PNNL, Richmond, WA*; ⁴*St. Peterburg Academic University, St. Peterburg, Russia*; ⁵*UCSD, La Jolla, CA*

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ThP 065 **Top-down Quantitative Proteomics Reveals Concerted Changes in Myofilaments in Ischemic Heart**; Ying Peng¹; Zachery Gregorich²; Santosh G Valeja³; Huseyin Guner¹; Yi-Chen (Ivy) Chen⁴; Timothy Hacker¹; Xiaowen Liu⁵; Ying Ge¹; ¹*University of Wisconsin - Madison, Madison, WI*; ²*UW Madison, Madison, WI*; ³*University of Wisconsin- Madison, MADISON, WI*; ⁴*University of Wisconsin-Madison, Madison, WI*; ⁵*IUPUI, Indianapolis, IN*

ThP 066 **Investigation of Instrumental Variables Effect on Intact Protein Multiple Reaction Monitoring Reproducibility in a Next Generation Triple Quadrupole Mass Spectrometer**; Evelyn Wang¹; Peter Combe²; Erin McAllister²; Kevin Schug¹; ¹*University of Texas at Arlington, Arlington, TX*; ²*Shimadzu Scientific Instruments, Columbia, MD*

ThP 067 **Characterization of Intact and Reduced Therapeutic Monoclonal Antibodies using Microflow Size Exclusion Chromatography Coupled with Mass Spectroscopy**; Khaled Mriziq¹; Xiang Zhu¹; Remco Van Soest¹; Eric Johansen²; Subodh Nimkar¹; ¹*SCIEX Separations, Division of AB SCIEX, Redwood City, CA*; ²*AB SCIEX, Redwood City, CA*

ThP 068 **NeuCode SILAC Enables Multiplexed Protein Quantitation From the Top Down**; Timothy W. Rhoads; Christopher M. Rose; Nicholas M. Riley; Derek J. Bailey; Anna E. Merrill; Alexander S. Hebert; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*

ThP 069 **Generalized Top-down Proteomics and Proteoform Analysis Platform with Wide and Narrow pI IEF-SPLC-MS**; Steven Patrie; *UT Southwestern Med. Center, Dallas, TX*

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ThP 070 **Differential Phosphoproteomic Profiling of Human Myogenesis using Stable Isotope Labeling by Amino acids (SILAC)**; Natarajan V Bhanu¹; Rosalynn Molden²; Zuofei Yuan¹; Benjamin A Garcia¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*Princeton University, Princeton, NJ*

ThP 071 **Hidden quantification – Obvious Modifications: Combining Metabolic Labeling with Top-Down Phospho- Proteomics using 2D Gel Electrophoresis (2D GE)**; Andreas Otto; Carolin Dewald; Christian Henschker; Michael Hecker; Dörte Becher; *University Greifswald, Greifswald, Germany*

ThP 072 **Identification of Potential Downstream Targets of a Histidine Phosphatase Domain of the General Transcription Factor IIIC**; Marco L. Hennrich¹; Nicholas M. I. Taylor²; Sebastian Glatt¹; Helga Groetsch¹; Anne-Claude Gavin¹; Christoph W. Mueller¹; ¹*EMBL Heidelberg, Heidelberg, Germany*; ²*Centro de Investigaciones Biologicas, Madrid, Spain*

ThP 073 **Demonstration of Orthogonal Complementary Enrichment Methods for Enhanced Phosphopeptide Profiling of Drug-Treated Gastric Carcinoma Cells**; Charles L. Farnsworth; Hongbo Gu; Xiaoying Jia; Kimberly Lee; Jian Min Ren; Jeffrey C. Silva; *Cell Signaling Technology, Danvers, MA*

ThP 074 **Dimethyl Labeling Approach to the Study of the TLR Response Pathway**; Art Nuccio; Nathan Manes; Virginie Sjoelund; Aleksandra Nita-Lazar; *NIH, Bethesda, MD*

ThP 075 **Meta-analysis of Arabidopsis Phospho-proteomics**; Klaas J. van Wijk¹; Giulia Friso¹; Dirk Walther²; Waltraud X. Schulze³; ¹*Cornell University, Ithaca, NY*; ²*Max Planck Institute for Plant Physiology, Golm, Germany*; ³*Department of Plant Systems Biology, Stuttgart, Germany*

ThP 076 **Quantitative Analysis of Phosphoproteins During *Candida albicans* Hyphal Formation**; Susan T. Weintraub¹; Kevin Hakala¹; Sammy Pardo¹; Brian C. Searle²; Derek Thomas³; ¹*UT Health Science Center at San Antonio, San Antonio, TX*; ²*Proteome Software Inc., Portland, OR*; ³*Grand Valley State University, Allendale, MI*

ThP 077 **Global Phosphoproteome Profiling For the Characterization of Escherichia Coli Strains**; Rabih Jabbour¹; Raja Sekhar Nirujogi³; Samir Deshpande^{2,2}; Mary Wade¹; A. Peter Snyder⁴; Akhilesh Pandey³; ¹*ECBC, Apg, MD*; ²*Science and Technology Corp., Edgewood, MD*; ³*Johns Hopkins University School of Medicine, Baltimore, MD*; ⁴*US Army /ECBC, Bel Air, MD*

ThP 078 **Development of Antibody-like Nanomaterials to Enrich Phosphoproteins for Proteome Analysis**; Leekyoung Hwang; Zachery R. Gregorich; Santosh G. Valeja; Serife A. Gunner; Wenxuan Cai; Song Jin; Ying Ge; *University of Wisconsin-Madison, Madison, WI*

- ThP 079 **A Sensitive Assay to Estimate Total Protein Phosphorylation Level in Complex Samples;** Li Pan; Jiazhen Zhang; Chuan-Chih Hsu; Linna Wang; Anton Iliuk; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
- ThP 080 **SILAC-based Quantitative Phosphoproteomics Identifies Substrates of Ser/Thr/Tyr Kinases and Phosphatases in *Bacillus Subtilis*;** Vaishnavi Ravikumar¹; Lei Shi²; Karsten Krug¹; Ivan Mijakovic^{2,3}; Boris Macek¹; ¹*Proteome Center Tuebingen, Tuebingen, Germany*; ²*AgroParisTech, Grignon, France*; ³*Chalmers University of Technology, Gothenburg, Sweden*
- ThP 081 **Quantitative Phosphoproteomics of STEK Cell Lines Implicates Novel Pathways in Pathogenesis of Fragile X Syndrome and Autism Spectrum Disorders;** Katarina Matic¹; Timo Eninger¹; Barbara Bardoni^{2,3}; Laetitia Davidovic^{2,3}; Boris Macek¹; ¹*Proteome Center Tuebingen, Tuebingen, Germany*; ²*Institut de Pharmacologie Moléculaire et Cellulaire, Valbonne, France*; ³*Université de Nice-Sophia Antipolis, Nice, France*
- ThP 082 **Quantitative Analysis of the Phosphoproteome Demonstrates Novel Roles of the O-GlcNAc Transferase in Modulating Cellular Signaling;** Jun Zhong; Marissa Martinez; Srana Sengupta; Albert Lee; Xinyan Wu; Raghothama Chaerkady; Robert O'Meally; Karen Reddy; Robert Cole; Akhilesh Pandey; Natasha Zachara; *Johns Hopkins University, Baltimore, MD*
- ThP 083 **-Omics Investigation of *Sulfolobus solfataricus* in Response to Different Carbon Sources;** Wen Qiu; Trong Khoa Pham; Phillip C. Wright; *Chelsi Institute, The University of Sheffield, Sheffield, UK*
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- ThP 084 **Characterization of Drug Mode-of-Action using Protein Stability Measurements;** M. Ariel Geer¹; Douglas H. Weitzel²; Do Yeon Kwon¹; Tesia N. Stephenson¹; Mark W. Dewhirst²; Jiyong Hong¹; Michael C. Fitzgerald¹; ¹*Duke University, Durham, NC*; ²*Duke University Medical Center, Durham, NC*
- ThP 085 **SILAC-Based Strategy for Proteome-Wide Thermodynamic Analysis of Protein-Ligand Binding Interactions;** Jagat Adhikari¹; Michael C. Fitzgerald^{1,2}; ¹*Duke Medical Center, Durham, NC*; ²*Duke University, Durham, NC*
- ThP 086 **The Effect of Mutations in beta-Amyloid on Zinc Ion Coordination;** Igor Popov^{1,2}; Maria Indeykina^{2,4}; Alexey Kononikhin^{1,2}; Sergey Kozin³; Eugene Nikolaev^{1,2}; ¹*Moscow Institute of Physics and Technology, Dolgoprudny, Russia*; ²*Emanuel Institute of Biochemical Physics, Moscow, Russia*; ³*Engelhardt Institute of Molecular Biology, Moscow, Russia*; ⁴*Institute for Energy Problems of Chemical Physics, Moscow, Russia*
- ThP 087 **Natural Products: A Promising Source for Potential β -Amyloid Inhibitors;** Anthony Tsaropoulos¹; Nikolaos Stavros Koulakiotis²; Dimitrios Anagnostopoulos³; Ioannis Kostakis⁴; ¹*University of Athens Medical School, Athens 115 27, Greece*; ²*University of Patras, Pharmacy Department, Patras 26504, Greece*; ³*The Goulandris Natural History Museum, Kifissia 145 62, Greece*; ⁴*University of Athens, Pharmacy Dpt., Athens 157 71, Greece*
- ThP 088 **Folding of Gaseous Protein Ions;** Fred W. McLafferty¹; Sergio Castro¹; Owen Skinner¹; Kathrin Breuker²; ¹*Cornell University, Ithaca, NY*; ²*University of Innsbruck, Innsbruck, Austria*
- ThP 089 **Unbiased Proteome-wide Interaction Analysis using Intracellular Protein Crosslinking;** Mark Larance; Kathryn Kirkwood; Thomas Crozier; Yasmeen Ahmad; Gareth Agius; Angus Lamond; *University of Dundee, Dundee, UK*
- ThP 090 **Evaluation of Gallium as a Tracer of Hemoglobin-Haptoglobin Complexes in Drug Delivery;** Shengsheng Xu; Rinat R. Abzalimov; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- ThP 091 **Proteomics Profiling of Target Complexes of Vorinostat using Chemical Probe and Mass Spectrometry Analysis;** Congcong Lu¹; Kai Zhang^{1,2}; Yi Zhang³; Minjia Tan³; ¹*Nankai University, department of chemistry, Tianjin, China*; ²*Tianjin Medical University, Tianjin, China*; ³*Shanghai Institute of Materia Medica, Shanghai, China*
- ThP 092 **Native Mass Spectrometry Analysis of the Novel Lipid-Binding Protein Mdm12;** Jiang Zhang; Andrew Young; Pascal Egea; Joseph A. Loo; *UCLA, Los Angeles, CA*
- ThP 093 **Probing Protein-Protein and Protein-DNA Interactions by Native Mass Spectrometry and Global Hydrogen Deuterium Exchange using Surface Acoustic Wave Nebulization (SAWN);** Lucas Monkkonen¹; Scott Heron²; Matthew Bush¹; Carlos Catalano¹; David Goodlett²; ¹*University of Washington, Seattle, WA*; ²*University of Maryland, Baltimore, MD*
- ThP 094 **Fast Online Solid-phase Extraction Frontend to Characterize Covalent and Non-covalent Interactions in Early Drug Discovery with Mass Spectrometry;** Pascal Bernet; Reto Brunner; Johannes Ottl; Christian Bergsdorf; *Novartis Institutes for BioMedical Research, Basel, Switzerland*
- ThP 095 **Real-time Native MS to Monitor the Effect of Point Mutations, Inhibitor or tRNA Binding on Tgt Subunitexchange and Dimer Stability;** Francois Debaene¹; Tran Xuan Phong Nguyen²; Frederick Ehrmann²; Alain Van Dorsselaer¹; Klaus Reuter²; Gerhard Klebe²; Sarah Cianferani¹; ¹*LSMBO, IPHC-DISA, Uds, CNRS, Strasbourg, France*; ²*Philipps-Universität Marburg, Marburg, Germany*
- ThP 096 **Improving the Reliability of Binding Constants Determined with Mass Spectrometry for Peptide-Zinc (II) Complexes;** Whitney A. Parrish; Allison S. Danell; *East Carolina University, Greenville, NC*
- ThP 097 **Semi-quantitative ESI-MS Assay for Screening Complex Oligosaccharides Mixtures against Proteins;** Elena Kitova; Amr El-Hawiet; John Klassen; *University of Alberta, Edmonton, Canada*
- ThP 098 **Novel Ligands for Human Noroviruses;** Ling Han¹; Elena Kitova¹; Ming Tan²; Xi Jiang²; John Klassen¹; ¹*University of Alberta, Edmonton, Canada*; ²*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*
- ThP 099 **Quantifying Protein-Carbohydrate Interactions Using Liquid Sample Desorption Electrospray Ionization Mass Spectrometry;** Yuyu Yao; Km Shams-Ud-Doha; Rambod Daneshfar; Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- ThP 100 **Enter Titleidentification of Novel E. coli Ribosome-Associated Proteins;** Suraj Saraswat; James P. Reilly; *Indiana University, Bloomington, IN*
- ThP 101 **AP-SWATH Dynamic Interactome of DJ-1 Under Oxidative Stress: Implications for Parkinson's Disease;** Bruno Manadas¹; Sandra Anjo¹; Matilde Melo¹; Liliã Loureiro¹; Lucia Sabala¹; José Carvalho^{1,2}; Vera Mendes¹; Tiago Faria²; Pedro Castanheira³; Rui Brito²; Mário Grãos³; ¹*Center for Neuroscience and Cell Biology, Cantanhede, Portugal*; ²*University of Coimbra, Coimbra, Coimbra, Portugal*; ³*Biocant - Innovation Center, Cantanhede, Portugal*
- ThP 102 **50 Ways to Leave Your Ligand: Finding Weak Interactions in a Fragment-Based Drug Discovery Screen;** Harry Sterling; Gavin Dollinger; *Novartis, San Francisco, CA*

- ThP 103 **An Improved AP/MS Platform for Identification of Extracellular Receptor-Ligand Interactions;** Xiaoting Tang¹; Sufen Shang¹; Mark Heipel¹; Joseph Kuijper¹; Cameron Brandt¹; Collin Hauskins¹; Asha Yabannavar¹; Vibeke Stennicke²; Wenfeng Xu¹; ¹Novo Nordisk Research Center, Seattle, WA; ²Novo Nordisk A/S, Måløv, Denmark
- ThP 104 **New method: Differential Enzymatic ¹⁶O/¹⁸O Labelling for the Identification of Cross-Linked DNA-protein Heteroconjugates;** Fiona Flett; C Logan Mackay; Heidrun Interthal; *University of Edinburgh, Edinburgh, UK*
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- ThP 105 **Importance of Lysine Residues in Huntington Exon 1 Aggregation: Analysis by HDX-MS-MS and Covalent Labeling LC-MS;** James Arndt; Maxmore Chaibva; Robert Brown; Kathleen Burke; Justin Legleiter; Stephen J. Valentine; *West Virginia University, Morgantown, WV*
- ThP 106 **Determining the Mode of Small Molecule Inhibition of Amyloid Formation from the Type-II Diabetes Related Peptide hIAPP using ESI-IMS-MS;** Lydia M. Young; Sheena E. Radford; Alison E. Ashcroft; *University of Leeds, Leeds, UK*
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- ThP 107 **Mass Spectrometry Reveals Chemically Induced Structural Changes of Protein G' by Which Intact Immune Complexes are Released from Affinity Columns;** Yelena Yefremova¹; Mahmoud Al-Majdoub¹; Kwabena F.M. Opuni¹; Cornelia Koy¹; Yuetian Yan²; Michael Gross²; Michael O. Glocker¹; ¹Proteome Center Rostock, University of Rostock, Rostock, Germany; ²Washington University in St. Louis, St. Louis, MO
- ThP 108 **Monitoring Dynamic Solvent-Induced Protein Unfolding by ESI-MS;** Michael Cammarata; Ryan Parker; Jennifer Brodbelt; *University of Texas, Austin, TX*
- ThP 109 **Determination of Structural and Dynamic Changes in Different Misfolded Forms of Superoxide Dismutase (SOD1) by Hydrogen Deuterium Exchange Mass Spectrometry;** Xiaobin Xu; Sheng Gu; Fang Qian; Paul Weinreb; Dingyi Wen; *Biogen Idec, Cambridge, MA*
- ThP 110 **Analysis of Intact Native Proteins by UVPD and ETD to Reveal Structural Information in the Gas Phase;** Michael Cammarata; Jennifer Brodbelt; *University of Texas, Austin, TX*
- ThP 111 **Dynamics Analysis of Ribosome Structure using 1 mg Cell Revealed by H/D Exchange;** Tatsuya Yamamoto^{1, 2}; Yasuaki Kabe^{1, 2}; Makoto Suematsu^{1, 2}; ¹Keio University, Tokyo, Japan; ²ERATO, JST, Tokyo, Japan
- ThP 112 **Tandem-Mass-Tags as Sensors for Local Conformational Change during Activation of Coagulation Factor IX;** Eduard Ebberink¹; Mariëtte Boon-Spijker¹; Esther Bloem¹; Alexander Meijer^{1, 2}; Koen Mertens^{1, 2}; ¹Department of Plasma Proteins, Sanquin, Amsterdam, The Netherlands; ²Pharmaceutical Sciences, Utrecht University, Utrecht, The Netherlands
- ThP 113 **Covalent Fragments from SID Fragmentation of the Helical Protein ROP Correlate with Precursor Secondary Structure;** Lindsay Morrison; Thomas Magliery; Vicki Wysocki; *Ohio State University, Columbus, OH*
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- ThP 114 **Identifying Metal-bound Histidine Residues Using Hydrogen Deuterium Exchange and Mass Spectrometry;** Katie Love; Jia Dong; Nicholas Borotto; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- ThP 115 **Examining the Complementary Nature of Hydrogen/Deuterium Exchange and Covalent Labeling through the Structural Analysis of β 2-Microglobulin;** Nicholas Borotto¹; Vanessa Mendoza²; Richard Vachet¹; ¹University of Massachusetts, Amherst, MA; ²Boston University, Boston, MA
- ThP 116 **Characterization of Transferrin Receptor Binding Mechanism throughout Endocytosis by Hydrogen Exchange and Electron Capture Dissociation;** Hanwei Zhao; Cedric E. Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- ThP 117 **High Sensitivity HX-MS² for Structure Function Studies of the Non-Homologous End Joining Complex;** Morgan Hoepfner; Yaping Yu; Martial Rey; Susan Lees-Miller; David Schriemer; *University of Calgary, Calgary, CANADA*
- ThP 118 **HDXMS Study of the Interaction between ASB9 and Creatine Kinase;** Deepa Balasubramaniam; Jamie Schiffer; Jonathan Parnell; Elizabeth Komives; *UCSD, La Jolla, California*
- ThP 119 **HDX-MS Epitope Mapping of Hemagglutinin in Complex with Influenza Neutralizing Biomolecules;** Cristina Puchades; Otto Diefenbach; Eveline Sneekes-Vriese; Els Brinkman-Van der Linden; Başak Kükrer; Adrian Apetri; *Crucell Vaccine Institute, Leiden, The Netherlands*
- ThP 120 **Rationalizing Differences in Thermodynamic Stability of Immunoglobulins using shape Selective Mass Spectrometry and Hydrogen/Deuterium-Exchange;** Matthew Edgeworth¹; Jonathan Phillips²; David Lowe²; Daniel Higazi²; James Scrivens¹; ¹University of Warwick, Coventry, UK; ²MedImmune, Cambridge, UK
- ThP 121 **Dynamic Signatures of Thermal Adaptation in DNA Polymerases Observed by Hydrogen Exchange;** Daniel Deredge¹; Chin-Chi Liu²; Vince LiCata²; Patrick Wintrode¹; ¹University of Maryland, Baltimore, MD; ²Louisiana State University, Baton Rouge, LA
- ThP 122 **Comparing the Structure and Dynamics of Phosphatidylinositol-Specific Phospholipase C from Bacillus thuringiensis and Staphylococcus aureus;** Bhavna Jois²; Anne Gershenson³; Mary Roberts⁴; Patrick Wintrode¹; ¹University of Maryland, Baltimore, MD; ²University of Maryland Baltimore County, Baltimore, MD; ³University of Massachusetts at Amherst, Amherst, MA; ⁴Boston College, Chestnut Hill, MA
- ThP 123 **Beyond Structure Characterization: Structure Dynamics (Hydrogen Deuterium Exchange) Guided Biocatalyst Improvement;** Rui Zhang¹; Ugur Uzuner²; Su Sun¹; Joshua Yuan²; Susie Dai¹; ¹Office of the Texas State Chemist, Department of V, College Station, TX; ²Department of Plant Pathology and Microbiology, College Station, TX
- ThP 124 **Does Protein-Ligand Binding Generally Induce Reduced Deuteration Rates? Globin Oxygenation Studies Provide Insights Into HDX Fundamentals;** Modupeola Sowole; Lars Konermann; *Univ. of Western Ontario, London, ON*
- ThP 125 **Epitope mapping and Interrogation of Allosteric Changes in Protein-Ligand Interactions Enabled by Site-Specific, Sub-Second-Timescale HDX on an Integrated Microfluidic Device;** Diana Resetca¹; Sina Haftchenary²; Patrick Gunning²; Derek Wilson¹; ¹York University, Toronto, Canada; ²University of Toronto Mississauga, Mississauga, Canada
- ThP 126 **HDX MS Depicts Intrinsic Structural Rearrangements of RIG-I upon Sensing Viral RNA and ATP Hydrolysis;** Jie Zheng; Huiyee Yong; Nantika Panutdaporn; Chun Loong Ho; Xueming Dong; Xiaobao Bi; Chuanfa Liu; Dahai Luo; Kai Tang; *Nanyang Technological University, Singapore*

- ThP 127 **Estimation of Protein Folding Rates of Staphylococcal Nucleases and Ubiquitin using PEPS(Protein Equilibrium Population Snapshot)-HDX-ESI-MS; Rohana Liyanage;** Reece Ritter; Wesley Stites; Jennifer Gidden; Jackson O. Lay Jr; *University of Arkansas, Fayetteville, AR*
- ThP 128 **An Autoantibody Binding Epitope in ADAMTS13 Protease Identified by Hydrogen/Deuterium Exchange Mass Spectrometry;** Wenbing Hu¹; Veronica C. Casina²; Zhong-yuan Kan¹; Leland Mayne¹; X. Long Zheng²; S. Walter Englander¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*The Children's Hospital of Philadelphia, Philadelphia, PA*
- ThP 129 **Lysyl-tRNA Synthetase (KRS)-induced Conformational Changes to the 37-kDa Laminin Receptor Precursor (37LRP)-Nanodisc Complex Revealed by H/D Exchange FT-ICR MS;** Yeqing Tao¹; Pengfei Fang³; Nicolas L. Young²; Min Guo³; Alan G. Marshall²; ¹*Florida State University, Tallahassee, FL*; ²*NHMFL / FSU, Tallahassee, FL*; ³*The Scripps Research Institute, Jupiter, FL*
- ThP 130 **Insights into the Conformational Dynamics of Oxidized Cu, Zn Superoxide Dismutase (SOD1), an ALS-Associated Post-Translational Modification;** Jared R. Auclair^{1,2}; Roxana E. Iacob¹; Qian Liu²; Dagmar Ringe²; Gregory A. Petsko²; John R. Engen¹; Jeffrey N. Agar¹; ¹*Northeastern University, Boston, MA*; ²*Brandeis University, Waltham, MA*
- ThP 131 **Investigating Fatty Acid Amide Hydrolase Membrane Association by Hydrogen Deuterium Exchange Mass Spectrometry;** Brent Kochert; Michael Johnson; Alexandros Makriyannis; John Engen; *Northeastern University, Boston, MA*
- ThP 132 **Conformational Dynamics of the Src-family kinase Hck following HIV-1 Nef and Small Molecule Inhibitor Binding;** Jamie A. Moroco¹; Thomas E. Wales¹; Lori A. Emert-Sedlak²; Thomas E. Smithgall²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*University of Pittsburgh School of Medicine, Pittsburgh, PA*
- ThP 133 **Structural Basis of β -arrestin-mediated GPCR Signaling --- Structural Information of β 2AR- β -arr1 Complexes Revealed by Mass Spectrometry;** Kunhong Xiao¹; Arun Shukla¹; Sheng Li²; Xiao Jie Yao¹; Minjung Choi¹; Jiang Qian¹; Adi Blanc¹; Robert Lefkowitz³; ¹*Duke University Medical Center, Durham, NC*; ²*University of California at San Diego, La Jolla, CA*; ³*HHMI, Duke University Medical Center, Durham, NC*
- ThP 134 **Characterization of the Binding Interface between rFVIIIc Fusion Protein and the von Willebrand Factor by Hydrogen/Deuterium Exchange Mass Spectrometry;** George Bou-Assaf; Ekta Seth Chhabra; John Kulman; *Biogen Idec, Cambridge, MA*
- ThP 135 **Detecting Differences in Structure and Dynamics between Wild Type hGH and a Variant by Hydrogen/Deuterium Exchange Mass Spectrometry and ETD;** Signe Teuber Seger^{1,2}; Mette Dahl Andersen¹; Jens Breinholt¹; Johan Faber¹; Christine Bruun Schjødtt¹; Kasper D. Rand²; ¹*Novo Nordisk, Måløv, Denmark*; ²*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*
- ThP 136 **Probing the Conformational Dynamics and Regulation of Dynamin Function using HDX Mass Spectrometry;** Venkat Dharmarajan¹; Saipraveen Srinivasan²; Sandra Schmid²; Patrick Griffin¹; ¹*The Scripps Research Institute, Jupiter, FL*; ²*UT Southwestern Medical Center, Dallas, TX*
- ThP 137 **Characterization of PPAR γ Mutations on Protein Dynamics With HDX;** David Marciano¹; Scott Novick¹; Bruce Pascal¹; John Bruning²; Patrick Griffin¹; ¹*The Scripps Research Institute, Jupiter, FL*; ²*The University of Adelaide, Adelaide, Australia*
- ThP 138 **Hydrogen/deuterium Exchange Mass Spectrometry Study of a New PPAR Ligand;** Luana Oliveira dos Santos¹; Aline Villanova Bridi²; Ana Carolina Migliorini Figueira²; Fabio C Gozto¹; ¹*Institute of Chemistry - University of Campinas, Campinas, SP*; ²*Brazilian Biosciences National Laboratory, Campinas, SP*
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- ThP 140 **A Combined Glycomics and Glycoproteomics Approach to Study the N-glycoproteome of Human Cerebrospinal Fluid;** Arnaud Goyallon; Sophie Cholet; Christophe Junot; Francois Fenaille; *CEA, iBiTec-S, SPI, Gif Sur Yvette, FRANCE*
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- ThP 247 **Variable Carboxylation of Osteocalcin in Human Bone**; Timothy P. Cleland¹; Corinne Thomas¹; Caren M. Gundberg²; Deepak Vashishth¹; ¹Rensselaer Polytechnic Institute, Troy, NY; ²Yale University, New Haven, CT
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- ThP 275 **Temporal Phosphoproteomic Study on Estrogen Receptor-Dependent Cytotoxicity in Renal Cell Carcinoma;** Wei-Chi Ku¹; Zhi-Yu Liu^{1,2}; Chi-Jung Huang^{1,3}; Kuo-Chiang Chen³; Yen-Chieh Wang³; Shao-Kuan Chen³; Chih-Ming Lin³; ¹*Fu Jen Catholic University, New Taipei, Taiwan*; ²*National Taiwan University, Taipei, Taiwan*; ³*Cathay General Hospital, Taipei, Taiwan*
- ThP 276 **Comprehensive Proteomic Analysis of Cisplatin Sensitive and Resistant Epithelial Ovarian Cancer Tumor Cells Guided by Transcriptomics;** Elizabeth Nguyen¹; Kaisa Huhtinen¹; Youngah Goo²; Jussi Salmi¹; Riika Lund¹; Robert Moulder¹; Olli Carpen¹; Riita Lahesmaa¹; David Goodlett²; ¹*Turku Centre for Biotechnology, Turku, Finland*; ²*University of Maryland, Baltimore, MD*
- ThP 277 **Towards Mass Spectrometric Profiling of Urinary Bladder Cancer—Optimization of sample Preparation, Protein Extract Generation, In-Solution Digestion, and nanoESI-IMS-MSE Analysis;** Cornelia Koy¹; Gargee Mukherjee¹; Claudia Roewer¹; Samantha Wickramasekara²; Claudia S. Maier²; Chris Protzel³; Oliver Hakenberg³; Michael O. Glocker¹; ¹*Proteome Center Rostock, Rostock, Germany*; ²*Department of Chemistry, Oregon State University, Corvallis, OR*; ³*Urology Clinic and Polyclinic, University Medicine, Rostock, Germany*
- ThP 278 **Proteomic Analysis of Plasmodium Berghei Hepatic Stage Merosomes;** Raja Sekhar Nirujogi^{1,4}; Satish Mishra²; Photini Sinnis³; Akhilesh Pandey⁴; ¹*Institute of Bioinformatics, Bangalore, India*; ²*Central Drug Research Institute, Lucknow, UP, India*; ³*JHMRI, Johns Hopkins University, Baltimore, MD*; ⁴*Johns Hopkins University School of Medicine, Baltimore, MD*
- ThP 279 **Effect of Statins on the Proteome of Human Pancreatic Stellate Cells;** Nerea Cuevas Polo¹; Kevin Broadbelt¹; Darwin Conwell²; Hanno Steen¹; ¹*Harvard Medical School/Children's Hospital Boston, Boston, MA*; ²*Ohio State University Wexner Medical Center, Ohio, OH*
- ThP 280 **A Comprehensive Tumor Tissue Analysis in Glioblastoma: Towards Understanding the Pathophysiology of Tumor Progression;** Vadiraja B. Bhat¹; Maxime S. Heroux²; Marla A. Chesnik²; Mona Al-Gizawi²; Shama P. Mirza²; ¹*Agilent Technologies, Wilmington, DE*; ²*Medical College of Wisconsin, Milwaukee, WI*
- ThP 281 **Quantitative Profiling of protein Tyrosine Kinases In Human Cancer Cell Lines by Multiplexed Parallel Reaction Monitoring Assays;** Hye-Jung Kim^{1,2}; Ming Li³; Daniel C. Liebler^{1,2}; ¹*Department of Biochemistry, Vanderbilt University, Nashville, TN*; ²*Jim Ayers Institute, Vanderbilt-Ingram Center, Nashville, TN*; ³*Department of Biostatistics, Vanderbilt University, Nashville, TN*
- ThP 282 **Quantitative Analysis of the Synaptic Proteome in the Nucleus Accumbens in Schizophrenia;** Suhong Zhang¹; Stephanie Willard¹; Warren Bilker²; Karin Borgmann-Winter^{1,3}; Chang-Gyu Hahn¹; ¹*Univ of Pennsylvania Dept of Psychiatry, Philadelphia, PA*; ²*Univ of Penn Dept of Biostatistics and Epidemiology, Philadelphia, PA*; ³*Children's Hospital of Philadelphia, Philadelphia, PA*
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- ThP 284 **Urinary Proteomics in the Discovery of Candidate Protein Biomarkers in Type 1 Diabetes Cohort;** Moo-Jin Suh; Yanbao Yu; Karen Nelson; Ramana Madupu; Rembert Pieper; *J. Craig Venter Institute, Rockville, MD*
- ThP 285 **Development and Validation of an Analytical Method for Discovery of Biomarkers of Preterm Birth;** Tracey C. Fleischer; Chad L. Bradford; Ashoka D. Polpitiya; Jeff S. Flick; Trina Pugmire; Robert D. Severinsen; Iliia Ichetovkin; Durlin Hickok; J. Jay Boniface; *Sera Prognostics, Salt Lake City, UT*
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- ThP 287 **Evaluation of SWATH™ as a Diagnostic Tool for Bacterial Identification Using a Strain's Specific Library;** Sylvie Bourassa¹; Isabelle Kelly¹; Frederic Fournier¹; Benjamin Nehme¹; Daniel Defoy¹; Brigitte Simons²; Maurice Boissinot³; Michel Bergeron³; Arnaud Droit^{1,4}; ¹*Proteomics, CHU de Quebec Research Center, Quebec, Canada*; ²*AB SCIEX, Concord, ON*; ³*Infectiology, CHU de Quebec Research Center, Quebec, Qc*; ⁴*Molecular Medicine, Laval University, Quebec, Qc*
- ThP 288 **Multivariate Statistical Procedures Implemented within the Framework of Statistical Process Control to Evaluate Data Quality in LC MS/MS;** Michael Bereman; Gina Hilton; Emily Griffith; *North Carolina State University, Raleigh, NC*

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- ThP 290 **Classification of Breast Cancer Sub-types with Site-Specific Phosphorylation Changes;** Harsha P. Gunawardena¹; Jonathon O'Brien²; John A. Wrobel¹; Ling Xie¹; Xian Chen¹; ¹*Biochemistry & Biophysics, School of Medicine, UNC-Chapel Hill, NC*; ²*Biostatistics, Gillings School of Public Health, UNC-Chapel Hill, NC*
- ThP 291 **Comparative Tissue Proteomics of Microdissected Specimens for Biomarker Discover of Bladder Cancer;** Yi-Ting Chen¹; Chien-Lun Chen²; Ting Chung¹; Chih-Ching Wu¹; Jau-Song Yu¹; Yu-Sun Chang¹; ¹*Chang Gung*

- University, Taoyuan, Taiwan; ²Department of Urology, Chang Gung Memorial Hospital, Taoyuan, Taiwan
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- ThP 294 **Proteomics Profiling of Pancreatic Patient Tumors and Their Xenografts: a Case Study;** Bingwen Lu¹; Camino Menendez³; Pedro P. Lopez-Casas³; Peter Olson¹; David Shields²; Manuel Hidalgo³; Jeremy Myers¹; Kim Arndt¹; ¹Pfizer, Pearl River, NY; ²Pfizer, La Jolla, CA; ³Spanish National Cancer Research Center, Madrid, SP
- ThP 295 **Toward the Elucidation of Changes in Protein Ubiquitylation Correlating with Ovarian Cancer BRCA1 Clinical Subtypes;** Stefani Thomas¹; Ie-Ming Shih¹; Douglas Levine²; Zhen Zhang¹; Daniel Chan¹; Hui Zhang¹; ¹Johns Hopkins University, Baltimore, MD; ²Memorial Sloan Kettering Cancer Center, New York, NY
- ThP 296 **Two-Dimensional Liquid Chromatography Coupled to Mass Spectrometry for Proteomic Profiling of Paraffin Embedded Lung Tumor Tissues;** Nilini Ranbaduge; Ferdinando Cerciello; Joseph Amann; David Carbone; Vicki Wysocki; *The Ohio State University, Columbus, OH*
- ThP 297 **Stretch-Induced Proteomic Changes in Vascular Smooth Muscle Cells of Rat Portal Vein in Vivo;** Rui Zhu¹; Amani Al Outa²; Zein Farhat²; Firas Kobeissy²; Ramzi Sabra²; Asad Zeidan²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²American University of Beirut, Beirut, Lebanon
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- ThP 301 **Direct Monitoring of Cerebellar Phosphorylation Dynamics in a Kinase Knockout Mouse;** Eleonora Corradini^{1,2}; Raghavan Vallur^{3,4}; Linsey M. Raaijmakers^{1,2}; Susanne Feil³; Robert Feil³; Albert J. R. Heck^{1,2}; Arjen Scholten^{1,2}; ¹Utrecht University, Utrecht, The Netherlands; ²Netherlands Proteomics Centre, Utrecht, The Netherlands; ³University of Tübingen, Tübingen, Germany; ⁴German Center for Neurodegenerative diseases, Tübingen, Germany
- ThP 302 **DIART Tandem Mass Spectrometric Analysis Reveals Anti-Oxidant Signaling of Elderberry and Sutherlandia against Transient Cerebral Ischemia in Mice;** Hui Zhou^{1,2}; Zhe Qu^{1,2}; Jiankun Cui^{1,2}; Agnes Simonyi^{2,3}; Jilong Li⁴; Shuwei Li⁸; Victoria A. Engel^{1,2}; Shanyan Chen^{1,2}; Jianlin Cheng⁴; C. Michael Greenliet⁸; Andrew L. Thomas⁶; Kevin L. Fritsche⁷; William R. Folk³; Dennis B. Lubahn^{3,7}; Grace Y. Sun^{2,3}; Zecong Gu^{1,2}; ¹University of Missouri School of Medicine Patholog, Columbia, MO; ²MU SOM Center for Translational Neuroscience, Columbia, MO; ³University of Missouri School of Medicine Biochem, Columbia, MO; ⁴University of Missouri Computer Sci., Informatics, Columbia, MO; ⁵University of Missouri Department of Chemistry, Columbia, MO; ⁶University of Missouri Southwest Res. Center, Columbia, MO; ⁷University of Missouri Division of Animal Sciences, Columbia, MO; ⁸University of Maryland Chemistry and Biochemistry, College Park, MD
- ThP 303 **Proteomic Profiling of Pig Colon Mucosa to Study the Effect of Consuming Anthocyanin-Rich Purple-fleshed Potatoes;** Sridhar Radhakrishnan^{1,2}; Vadiraja Bhat³; Sungwoo Kim⁴; Andrey Ptitsyn⁵; Lavanya Reddivari⁶; Jairam Vanamala¹; ¹Colorado State University, Fort Collins, Colorado; ²Food Science, Penn State University, University Park, PA; ³Agilent Technologies, Wilmington, DE; ⁴Animal Science, North Carolina State University, Raleigh, North Carolina; ⁵Sidra Medical and Research Center, Doha, Qatar; ⁶Plant Science, Penn State University, State College, PA
- ThP 304 **Comparative Proteomic Analysis of Carbonylated Proteins from the Striatum and Cortex of Pesticide Treated Mice;** Christina Coughlan¹; Douglas Walker²; Kelly Loh³; Michael Caudle³; Kristofer Fritz¹; James Roede¹; ¹University of Colorado Anschutz Medical Campus, Aurora, CO; ²Tufts University, Medford, MA; ³Emory University, Atlanta, GA
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- ThP 306 **Multi-platform Data Integration of the Cerebral Cortex Proteome in Rodent Models of Fear Conditioning and Repetitive Blast;** Angela M. Boutte¹; Joy Guingab-Cagmat²; Eric Mauldin-Jeronimo³; Larry P. Simmons¹; Stephen T. Ahlers³; Raymond F. Genovese¹; Frank C. Tortella¹; Kara E. Schmid¹; Jitendra R. Dave¹; ¹Walter Reed Army Institute of Research, Silver Spring, MD; ²Banyan Biomarkers, Inc., Alachua, FL; ³Naval Medical Research Center, Silver Spring, MD
- ThP 307 **Proteomic Analysis of Liver in Rats with lead Exposure and Iron-Supplemented;** Mileni Silva Fernandes²; Aline Lima Leite²; Fernanda Zucki¹; Lucas Ferreira Almeida¹; Marília Afonso Rabelo Buzalaf¹; ¹USP-FOB, Bauru, BRAZIL; ²Federal University of São Carlos, São Carlos, SP
- ThP 308 **Proteomic MS analysis of FASP-Processed FFPE Leptomeningeal Amyloid Brain Tissue Identifies Transthyretin Where Immunohistochemical Staining Fails;** Anna Okumu¹; Michael Greicius²; Edward Plowey³; Yuxi Wu¹; Allis Chien¹; Chris Adams¹; ¹Stanford University Mass Spectrometry, Stanford, CA; ²Dept of Neurology, Stanford Univ. Sch. of Medicine, Stanford, CA; ³Dept of Pathology, Stanford Univ. Sch. of Medicine, Stanford, CA
- ThP 309 **Identification of Toluene Diisocyanate-Conjugated Murine Protein Targets following Dermal Exposures;** Justin M. Hettick; Ajay P. Nayak; Carrie M. Long; Stacey E. Anderson; Paul D. Siegel; *NIOSH, Morgantown, WV*
- ThP 310 **Novel Proteogenomic Analysis Establishes the Sea Star *Patiria miniata* as a New Systems Biology Model for Neuronal Regeneration;** Catarina Franco^{1,2}; Michael Sweredoski²; Parul Kudtarkar³; R. Andrew Cameron³; Sonja Hess²; ¹Instituto de Tecnologia Química e Biológica, Oeiras, Portugal; ²Proteome Exploration Laboratory, Caltech, Pasadena, CA; ³Center for Computational Regulatory Genomics, Caltech, CA
- ThP 311 **In-Depth Proteomic Analysis of Human Substantia Nigra;** Chan-Hyun Na; *Johns Hopkins University School of Medicine, Baltimore, MD*

- ThP 312 **Comparative Proteome Analysis of Porcine Placenta between Small and Large Litter Size Groups;** Dong-Gi Lee¹; Young-Moon Kang^{1,4}; Sang-Je Park²; Hwa Chun Park³; Chul Wook Kim²; Jong-Soon Choi^{1,4}; ¹*Korea Basic Science Institute, Daejeon, South Korea*; ²*Gyeongnam National University of Science and Techn, Jinju, South Korea*; ³*Dasan Genetics, Namwon, South Korea*; ⁴*GRAST, Chungnam National University, Daejeon, South Korea*
- ThP 313 **Mass Spectrometry-based Proteomics of Human Induced Pluripotent Stem Cells (hiPSC) Cultured in Suboptimal Culture Conditions;** Melkamu Getie-Kebtie¹; Natalia Pripuzova¹; Christopher Grunseich²; Colin Sweeney³; Harry Malech³; Michail Alterman¹; ¹*Division of Cell and Gene Therapy, CBER, FDA, Bethesda, MD*; ²*Neurogenetics Branch, NINDS, NIH, Bethesda, MD*; ³*Laboratory of Host Defenses, NIAID, NIH, Bethesda, MD*
- ThP 314 **Phosphoproteomic Analysis Reveals Regulatory Mechanisms at the Kidney Filtration Barrier;** Markus Rinschen¹; Xiongwu Wu²; Tim König³; Trairak Pisitkun⁴; Bernard Brooks²; Pedro Beltrao⁵; Marcus Krüger⁶; Paul Brinkkötter¹; Thomas Benzinger¹; ¹*Internal Medicine II, University Hospital Cologne, Koeln, Germany*; ²*NIH, NHLBI, Bethesda, MD*; ³*CECAD, Cologne, Germany*; ⁴*Chulalongkorn University, Bangkok, Thailand*; ⁵*EMBL, EBI, Hinxton, Cambridge, UK*; ⁶*MPI Bad Nauheim, Bad Nauheim, Germany*
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- ThP 316 **Exploring Impact of Dynamic Accumulation for Improving MS/MS Quality of QqTOF Data;** Aaron Hudson¹; Christie Hunter²; Sean L. Seymour³; Nic Bloomfield¹; ¹*AB SCIEX, Framingham, MA*; ²*AB SCIEX, Foster City, CA*; ³*AB SCIEX, Redwood City, CA*
- ThP 317 **In-Depth Proteome Coverage by Iterative Data Dependent Acquisition on a Benchtop Orbitrap Mass Spectrometer;** Mathias Mueller; Tabiwang N. Arrey; Thomas Rietpietsch; Florian Grosse-Coosmann; Andreas Kuehn; Catharina Crone; Torsten Ueckert; Markus Kellmann; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- ThP 318 **Comparison of Data-Dependent Acquisition (DDA) and Data-Independent Acquisition (DIA) Strategies in Discovery and Label-Free Quantitation of a Complex Proteome;** Suresh Annangudi; David McCaskill; Jeffrey Gilbert; *Dow Agrosciences, Indianapolis, IN*
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- ThP 320 **MS³-based Quantitative Proteomics using Pulsed-Q Dissociation (PQD);** Zhiyun Cao; Adam R. Evans; Renã A. S. Robinson; *University of Pittsburgh, Pittsburgh, PA*
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- ThP 324 **Evaluation of Data-Independent Acquisition (DIA) Approaches for Spiked Peptides in HeLa Digest on Q-OT-qIT Mass Spectrometer;** Wei Zhang¹; Reiko Kiyonami²; Zheng Jiang¹; Wei Chen¹; ¹*ThermoFisher Scientific, Shanghai, CHINA*; ²*ThermoFisher Scientific, San Jose, CA*
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- ThP 326 **An Approach for Peptide Identification Combining DDA and DIA on a Q Exactive Plus Prototype with a High-Field Orbitrap;** Han-Yin Yang; Jarrett Egertson; Jennifer Merrihew; Michael J. Maccoss; *Univ of Washington, Seattle, WA*
- ThP 327 **NeuCode + SWATH = a Good Combination;** Alicia Richards; Catherine E. Minogue; Alex Hebert; Jarred W. Rensvold; Anna Merrill; Allison Balloon; Michael S. Westphall; Audrey P. Gasch; David J. Pagliarini; Joshua J. Coon; *University of Wisconsin, Madison, WI*
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- ThP 329 **Combination of DDA, DIA and Targeted Approaches for the Analysis of Protein-Metabolite Interactions using Proteolytic Probes and an Orbitrap Fusion;** Paolo Nanni¹; Paul Boersema²; Yuehan Feng²; Christian Trachsel¹; Nathalie Selevsek¹; Paola Picotti²; Ralph Schlapbach¹; ¹*University/ETH Zurich - FGCZ, Zurich, Switzerland*; ²*ETH Zurich, Dept Biology, Institute of Biochemistry, Zurich, Switzerland*
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- ThP 355 **Uncovering Biomolecular Structure at Single Residue Resolution using Mass Spectrometry Based Covalent Labeling**; Parminder Kaur^{1,2}; Janna Kiselar¹; Giridharan Gokulrangan¹; Mark Chance^{1,2}; ¹Case Western Reserve University, *Cleveland, OH*; ²NeoProteomics, *Inc., Cleveland, OH*
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- ThP 358 **Promoting Ozonolysis for Protein Footprinting by Radical Probe Mass Spectrometry**; Simin D. Maleknia¹; Keith Fisher²; ¹University of New South Wales, *Sydney, Australia*; ²University of Sydney, *Sydney, Australia*

- ThP 359 **Covalent-labeling Strategy for the Thermodynamic Analysis of Protein Folding and Ligand Binding in Complex Mixtures;** Yingrong Xu¹; Erin C. Strickland^{1,2}; Emily R. Derbyshire¹; Michael C. Fitzgerald¹; ¹Duke University, Durham, NC; ²Current Address: Ameritox, Greensboro, NC
- ThP 360 **Differential Surface Modification under Denaturing And Native Conditions for the Identification of Surface-Exposed Amino Acid Residues in Alpha-Synuclein;** Nicole Sessler¹; Nicholas Brodie¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 361 **Structural Proteomic Analysis of SOD1 Aggregation;** Nicholas Brodie¹; Evgeniy Petrotchenko¹; Christoph Borchers^{1,2}; ¹University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; ²UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 362 **Conformational Analysis of Intrinsically Disordered Proteins by Fast Photochemical Oxidation of Proteins;** Mohammed Al-Naqshabandi^{1,2}; Hao Zhang³; Ben Niu³; Michael L. Gross³; David Weis¹; ¹University of Kansas, Lawrence, KS; ²University of Soran, Erbil, Iraq; ³Washington University, St Louis, MO
- ThP 363 **Probing Conformational Changes in Amyloid Beta Aggregation by Fast Photochemical Oxidation of Proteins (FPOP);** Ke Sherry Li; Ying Zhang; Don L. Rempel; Michael L. Gross; *Department of Chemistry, Washington University, St. Louis, MO*
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- ThP 364 **A Laser Desorption Mass Spectroscopy Study of Titan Aerosol Analogs Formed from Aromatic Precursors;** Melissa Trainer¹; Joshua Sebree²; Xiang Li¹; Veronica Pinnick¹; Stephanie Getty¹; William Brinckerhoff¹; ¹NASA, Greenbelt, MD; ²University of Northern Iowa, Cedar Falls, IA
- ThP 365 **In Situ Analysis of Organics on Planetary Surfaces by Miniature Two-Step Laser Time-of-Flight Mass Spectrometer;** Xiang Li¹; Stephanie Getty²; William Brinckerhoff²; Timothy Cornish³; Scott Ecelberger³; Melissa Floyd²; Qinghao Wu⁴; Richard Zare⁴; Jamie Elsil Cook²; ¹University of Maryland, Baltimore County, Baltimore, MD; ²NASA GSFC, Greenbelt, MD; ³C&E Research, Inc., Columbia, MD; ⁴Stanford University, Stanford, CA
- ThP 366 **The Identification of Biosignatures on Planetary Surfaces from in situ Techniques, Including Miniaturized Mass Spectroscopy;** Kyle Uckert¹; Nancy J. Chanover¹; Stephanie Getty²; William B. Brinckerhoff²; David G. Voelz¹; Nancy McMillan¹; Xifeng Xiao¹; Xiang Li³; Mellisa Floyd²; Penelope J. Boston⁴; ¹New Mexico State University, Las Cruces, NM; ²NASA GSFC, Greenbelt, MD; ³University of Maryland, Baltimore County, Greenbelt, MD; ⁴New Mexico Institute of Mining and Technology, Socorro, NM
- ThP 367 **Molecular Composition and Optical Properties of Organo-Nitrogen Species in Organic Aerosol;** Chris Stangl; Murray Johnston; *University of Delaware, Newark, DE*
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- ThP 370 **Survivability of Electrospayed Bacterial Spores upon High-Velocity Surface Impact;** Brandon L Barney; Kit Anderson; Daniel E Austin; *Brigham Young University, Provo, UT*
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- ThP 375 **Lipidome Analysis of Plasma, Livers, And Adipose Tissues in High-Fat-Diet-Fed Mice Using Supercritical Fluid Chromatography Coupled to High-Resolution Mass Spectrometry;** Takayuki Yamada¹; Yoshihiro Izumi¹; Shin Nishiumi²; Masaru Yoshida²; Eiichiro Fukusaki¹; Takeshi Bamba¹; ¹Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, Japan; ²Div. Gastro., Kobe Univ. Grad. Sch. Med., Kobe, Japan
- ThP 376 **Alterations of Lipid Metabolism in Preeclampsia: Lipid Characterization in the Maternal Circulation and Placenta;** Simon Brown¹; Samuel Eather¹; Dilys Freeman²; Barbara Meyer¹; Todd W Mitchell¹; ¹University of Wollongong, Wollongong, Australia; ²University of Glasgow, Glasgow, UK
- ThP 377 **Understanding the Role of Lipids during the Embryonic Development of the American Alligator (Alligator mississippiensis) using a Lipidomics Approach;** Stephen Somerville¹; John Bowden²; Theresa Cantu¹; Louis J. Guillette, Jr. ¹; ¹Medical University of South Carolina, Charleston, SC; ²NIST, Charleston, SC
- ThP 378 **Supercritical Fluid Chromatography Coupled to Mass Spectrometry for Comprehensive Bile Acid Profiling;** Kaori Taguchi; Eiichiro Fukusaki; Takeshi Bamba; *Graduate school of engineering, Osaka university, Suita, Japan*
- ThP 379 **Characterization of Human Cancer Cell Lines Using Rapid Evaporative Ionization Mass Spectrometry;** Nicole Strittmatter¹; Anna Lovrics²; Emrys A Jones¹; Ottmar Golf¹; Kirill Veselkov¹; Gergely Szakacs²; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Hungarian Academy of Sciences, Budapest, Hungary
- ThP 380 **Lipogenesis in Adipocyte using Isotope Tracer Mass Spectrometry;** Fereshteh Zandkarimi; Claudia S. Maier; *Chemistry Department of Oregon State University, Corvallis, OR*
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- ThP 383 **Direct Identification of Omega-3/6 Fatty Acid Incorporated Phosphatidylcholine in Mouse Serum and Tissue by MALDI-MS and LC-MS Based Metabolic Profiling;** Lin Tan; Patrea Rhea; Peiyang Yang; *MD Anderson Cancer Center, Houston, TX*
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- ThP 386 **Angiotensin Converting Enzyme Regulates the Lipid Composition of Macrophages**; Bogdan-Gabriel Gugiu¹; Teresa Hong¹; Kenneth Bernstein²; Markus Kalkum¹; ¹*City of Hope, Duarte, CA*; ²*Cedars-Sinai Medical Center, Los Angeles, CA*
- ThP 387 **Ethanol Induced Quantitative Brain Lipid Changes in Mice**; Aurelie Roux¹; Shelley N Jackson¹; Ludovic Muller^{1,2}; Joseph R. O'Rourke³; Panayotis K. Thanos³; Nora D. Volkow¹; Amina S. Woods¹; ¹*NIDA-IRP, NIH, Baltimore, MD*; ²*University of Pittsburgh, Pittsburgh, PA*; ³*Stony Brook University, Stony Brook, NY*
- ThP 388 **Multivariate Analyses of Phospholipids in Normal and Ischemic Rat Brain Parenchyma**; Hay-Yan J. Wang¹; Hsuan-Wen Wu¹; Zhi-Fu Zheng¹; Ping-Ju Tsai²; Cheng Bin Liu^{1,3}; ¹*National Sun Yat-Sen University, Kaohsiung, TAIWAN*; ²*Yuan's General Hospital, Kaohsiung, Taiwan*; ³*Veterans General Hospital-Kaohsiung, Kaohsiung, Taiwan*
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- ThP 391 **Cerebrospinal Fluid and Plasma Lipid Profiling using High Resolution Mass Spectrometry and Integrated Data Processing Tools**; Benoit Colsch¹; Alexandre Seyer²; Samia Boudah¹; Simon Broudin²; Christophe Junot¹; ¹*CEA de SACLAY, Gif Sur Yvette Cedex, France*; ²*Profilomic SA, Boulogne-Billancourt, France*
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- ThP 393 **Lipidomic Analysis of Different Cotton Seed Oil Genotypes Using Novel Analytical and Informatics Tools**; Vladimir Shulaev¹; Michael Jones²; Drew Sturtevant¹; Patrick Horn¹; Janna Crossley¹; Kent Chapman¹; James Langridge³; Giorgis Isaac²; ¹*University of North Texas, Denton, TX*; ²*Waters Corporation, Milford, MA*; ³*Waters Corporation, Manchester, UK*
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- ThP 398 **A Comprehensive Monitoring Method for lipid Mediators using a High-Speed LC/MS with Continuous Ionization Polarity Switching**; Masaki Yamada^{1,2}; Yoshihiro Kita¹; Takahiro Kohira^{1,3}; Suzumi Tokuoaka¹; Takao Shimizu^{1,4}; ¹*The University of Tokyo, Tokyo, JAPAN*; ²*Shimadzu Corporation, Kyoto, Japan*; ³*Japanese Red Cross Society, Tokyo, Japan*; ⁴*National Center for Global Health and Medicine, Tokyo, Japan*
- ThP 399 **Shotgun Fatty Acidomics Analysis of Eicosanoids in Biological Samples by Charge-Remote Fragmentation Approaches**; Miao Wang; Chunyan Wang; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*
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- ThP 402 **Quantitative Analysis of Bile Acids and Taurine Conjugates in Mouse Plasma Using a High Resolution Accurate Mass Approach**; Shunyan Mo; Karin Green; Timothy P. Fitzgibbons; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*
- ThP 403 **High Throughput and High Sensitivity LC-MS/MS Analysis of GM1 and GM2 Gangliosides in Brain**; Karin Green; Cara M. Weismann; Miguel Sena Esteves; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*
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- ThP 406 **Improving Lipid Profiling Performance using MicroFlow Liquid Chromatography and High Resolution Mass Spectrometry**; Jinyuan Wang¹; Baljit Ubhi¹; Christie Hunter¹; Anthony Romanelli²; Alexander Chassy³; Tomas Cajka³; Oliver Fiehn³; ¹*AB SCIEX, Redwood City, CA*; ²*AB SCIEX, Framingham, MA*; ³*UC Davis, Davis, CA*
- ThP 407 **Qualitative and Quantitative Analysis of Oxidized Fatty Acids by Information Dependent and Data Independent Strategies on a QTOF Instrument**; Xu Wang¹; Priscilla BMC Derogis²; Sayuri Miyamoto²; Sahana Mollah³; Christie Hunter³; ¹*AB SCIEX, Framingham, MA*; ²*Instituto de Química - Universidade de São Paulo, São Paulo, Brazil*; ³*AB SCIEX, Redwood City, CA*
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- ThP 410 **Supercritical Fluid Chromatography - Electrospray Ionization Mass Spectrometry as a Novel Approach for Fast and Complex Lipidomic Characterization**; Michal Holcapek; Miroslav Lisa; University of Pardubice, Pardubice, Czech Republic
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- ThP 496 **Simultaneous Quantification of Acridinium and its Metabolites in Human Plasma using LC-MS/MS Coupled with SelexION™ Technology;** Qingguo Tian¹; Haodan Yuan¹; Jordi Aubets²; Josep Jansat²; Daksha Desai-Krieger¹; Andreas Grill¹; ¹Forest Laboratories, Inc., Farmingdale, NY; ²Almirall S.A., Sant Feliu de Llobregat, Spain
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- ThP 591 **Rapid and Simple Determination of Benzodiazepines, Zolpidem and Their Metabolites using Direct Injection Liquid Chromatography-Tandem Mass Spectrometry;** Yu-Dong Jeong¹; Sunglll Suh²; Moon Kyo In²; Junghan Song³; Jin Young Kim²; Ki-Jung Paeng¹; ¹Yonsei University, Wonju, South Korea; ²Supreme Prosecutors' office, Seoul, South Korea; ³Seoul National University Bundang Hospital, Bundang, South Korea
- ThP 592 **Simultaneous Analysis for Forensic Drugs in Human Blood and Urine using Ultra-High Speed LC-MS/MS;** Toshikazu Minohata¹; Keiko Kudo²; Kiyotaka Usui³; Noriaki Shima⁴; Munehiro Katagi⁴; Noriaki Ikeda²; Hitoshi Tsuchihashi⁵; Koichi Suzuki⁵; ¹Shimadzu Corporation, Kyoto, Japan; ²Kyushu University, Fukuoka, Japan; ³Tohoku University Graduate School of Medicine, Sendai, Japan; ⁴Osaka Prefectural Police, Osaka, Japan; ⁵Osaka Medical Collage, Takatsuki, Japan
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- ThP 599 **Determination of Opiates, Amphetamines and Cocaine in Whole Blood, Plasma and Urine by UHPLC-MS/MS using a QuEChERS Sample Preparation;** Sylvain Dulaurent²; Mikael Levi¹; Jean-Michel Gaulier²; Stephane Moreau³; Pierre Marquet^{2,4}; ¹Shimadzu France, Noisiel, France; ²CHU Limoges, Department of Pharmacology and Toxicology, Limoges, France; ³Shimadzu Europe, Albert-Hahn Strasse 6-10, Duisburg, Germany; ⁴Univ Limoges, Limoges, France
- ThP 600 **Determination of Δ9-tetrahydrocannabinol and Two of its Metabolites in Whole Blood, Plasma and Urine by UHPLC-MS/MS using QuEChERS Sample Preparation;** Sylvain Dulaurent¹; Mikael Levi²; Jean-Michel Gaulier¹; Stephane Moreau³; Pierre Marquet^{1,4}; ¹Chu Limoges, Department of Pharmacology and Toxicology, Limoges, France; ²ShimadzuFrance, Noisiel, France; ³Shimadzu Europe, Albert-Hahn Strasse 6-10, Duisburg, Germany; ⁴Univ Limoges, Limoges, France
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- ThP 678 **Ketamine CYP3A Mediated Metabolism Study using Mammalian Liver S9 Fractions, cDNA Expressed Enzymes and Liquid Chromatography Tandem Mass Spectrometry;** [Raphaël Santamaria](#); Floriane Pailleux; Francis Beaudry; *Université de Montréal, St-Hyacinthe, CANADA*
- ThP 679 **Comparative Cellular Pharmacology of a β -D-2'-C-methyl-2,6-diaminopurine ribonucleoside phosphoramidate RS-1389 with INX189 and IDX184 in Rat, Dog, Monkey and Human Hepatocytes;** [Sijia Tao](#)¹; Longhu Zhou¹; Shaoman Zhou¹; Jong-Hyun Cho¹; Steven J. Coats²; Raymond F. Schinazi¹; ¹*Emory University School of Medicine, Atlanta, GA*; ²*RFS Pharma LLC, Tucker, GA*
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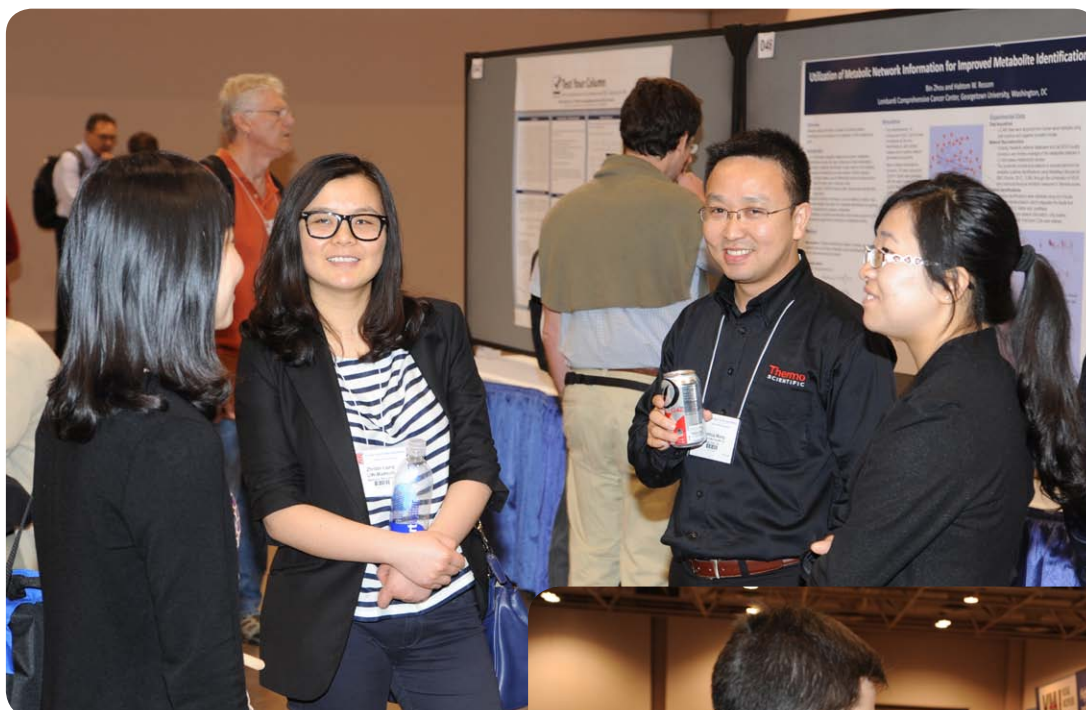
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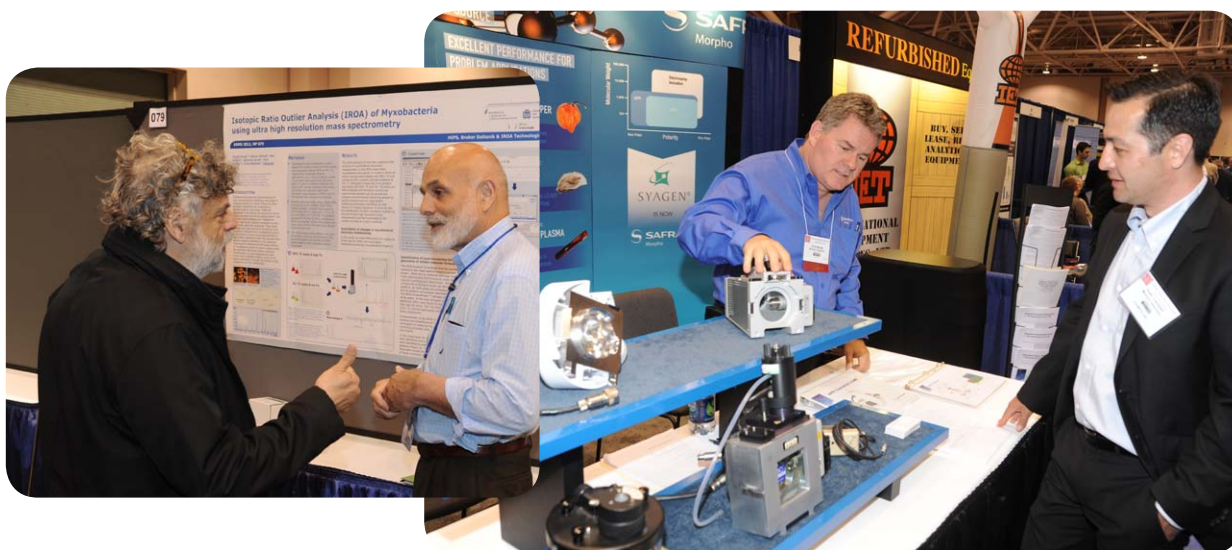
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