



Unravelling the color of a worldwide Rosé wine collection by UHPLC-MRM-MS polyphenol profiling

Nicolas Sommerer, Marine Lambert, Arnaud Verbaere, Emmanuelle Meudec, Marie-Agnès Ducasse, Jean Claude Boulet, Gerard Mazerolles, Gilles Masson, Veronique Cheynier

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Welcome to the 64th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Henry B. Gonzalez Convention Center. Corporate Member hospitality suites are located in the Grand Hyatt Hotel.

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GENERAL INFORMATION

REGISTRATION is open 1:00 - 5:00 pm on Saturday, 10:00 am - 8:00 pm on Sunday, and 7:30 am - 5:00 pm on Monday - Thursday.

ATTENTION UNDERGRADUATE STUDENTS AND FIRST TIME (AT ASMS) GRADUATE STUDENTS

4:00 - 5:00 pm, Sunday, Stars Ballroom 1, level 3

Plan Your Strategy: What to See and Do at ASMS

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

Hall 1, level 1

5:00 - 5:45 pm

Forensic Mass Spectrometry

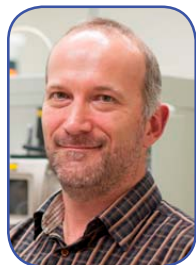
#TellMeSomethingIDontKnow



Facundo Fernandez
Georgia Institute of Technology



Glen Jackson
West Virginia University



5:45 - 6:30 pm

An Analyte's Journey from Solution into the Gas Phase

Lars Konermann
University of Western Ontario

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

Hall 1, level 1



Welcome

Vicki H. Wysocki
The Ohio State University
ASMS Vice President for Programs



A Molecular Arsenal Against Ebola Virus

Erica Ollmann Saphire
The Scripps Institute-La Jolla

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

Poster/Exhibit Hall. Conference name badge is required.

PLENARY SESSIONS

MONDAY AWARD LECTURE, 4:45 - 5:30 PM

Hall 1, level 1



Award for a Distinguished Contribution in Mass Spectrometry

Scott A. McLuckey
Purdue University

TUESDAY AWARD LECTURE, 4:45 - 5:30 PM

Hall 1, level 1



Biemann Medal

Kristina Håkansson
University of Michigan

THURSDAY PLENARY LECTURE, 4:45 - 5:30 PM

Hall 1, level 1



More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds

William Bialek
Princeton University

DON'T MISS

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

Stars Ballroom 1, level 3

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

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

Briscoe Western Art Museum

Let's celebrate! Stroll to the Briscoe for a western barbecue under the live oak trees of the terrace overlooking the San Antonio Riverwalk. View the exhibits which preserve and interpret the art, history, and culture of the American West. The evening continues with music, dancing and karaoke. Ticket is required, \$30.





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

Level 1

Session A (MOA, TOA, WOA, ThOA) Hall 1

Level 2

Session B (MOB, TOB, WOB, ThOB)..... Room 221

Level 3

Session C (MOC, TOC, WOC, ThOC)..... Stars 1

Session D (MOD, TOD, WOD, ThOD)..... Stars 2-3

Session E (MOE, TOE, WOE, ThOE)..... Stars 4

Session F (MOF, TOF, WOF, ThOF)..... Hemisfair 3

Session G (MOG, TOG, WOG, ThOG)..... Hemisfair 2

Session H (MOH, TOH, WOH, ThOH)..... Hemisfair 1

ORAL PRESENTATIONS are projected from ASMS computers running Microsoft Office. 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 222, level 2. The room is open with a technician according to this schedule:

Sunday: 10:00 am - 8:00 pm

Monday through Thursday: 7:30 am - 2:00 pm

POSTERS AND EXHIBIT BOOTHS are in the Poster/Exhibit Hall. 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. **Refer to the poster numbers in this final program for board assignments.** A counter for poster supplies is near the main entrance to the Hall.

POSTER SESSIONS are 10:30 am - 2:30 pm, Monday through Thursday.

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

10:30 am - 1:00 pm Odd-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 - Thursday 10:30 am - 2:30 pm

WORKSHOPS are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function areas on level 2 and 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

- **Sunday, 7:30 - 9:00 pm, Poster competition,** Poster/Exhibit Hall
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** Lunch tables reserved for undergraduate students in the Poster/Exhibit Hall. Free vouchers for lunch will be provided at the tables. Arrive promptly at 11:30 am to obtain your voucher.

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. 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 an extended abstract.**

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 and login. The link to "web casting" is on the annual conference page.

CORPORATE HOSPITALITY SUITES are open to all attendees from at least 8:00 - 11:00 pm Monday - Wednesday. Suites are also open during the day for one-on-one or small group meetings (no more than 25 people) by appointment only. Interested attendees should contact their sales representative for more information. Companies may also use their suites for breakfast seminars. Suites are located in the **Grand Hyatt 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 rooms must be reserved one day in advance.

Sunday7:45 - 9:00 pm

Monday - Wednesday7:30 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.

SINGLE USE/FAMILY RESTROOMS are available on each level.

MOTHER'S ROOM is Room 215 (for mothers only). From the Ballroom Level proceed to the Hemisfair Ballroom foyer and take escalators down. Room 215 is on the right side of the foyer space.

GENERAL INFORMATION

CORPORATE BREAKFAST SEMINARS are located in the convention center and at the Grand Hyatt. Reservations are required and may be made at company exhibit booths.

MONDAY	
Company	Convention Center Room
Advanced Chemistry Development	Room 224
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Bruker Daltonics	Room 225CD
LECO	Room 303A
Matrix Science	Room 302BC
SCIEX	Room 304A
SCIEX	Room 305
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
Waters Corporation	Room 301A
TUESDAY	
Company	Convention Center Room
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Biotage	Room 225B
Bruker Daltonics	Room 225CD
GL Sciences	Room 301A
LECO	Room 303A
Matrix Science	Room 302BC
MilliporeSigma	Room 303BC
New Objective	Room 305
Prosolia	Room 224
SCIEX	Room 302A
SCIEX	Room 304A
SCIEX	Room 304BC
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
WEDNESDAY	
Company	Convention Center Room
Agilent Technologies (at Grand Hyatt)	Lone Star Ballroom DEF
Bruker Daltonics	Room 225CD
LECO	Room 303A
New Objective	Room 305
SCIEX	Room 302A
SCIEX	Room 304A
SCIEX	Room 304BC
Shimadzu	Room 220
Thermo Fisher Scientific (at Grand Hyatt)	Republic ABC
Waters Corporation (at Grand Hyatt)	Texas Ballroom BC
Waters Corporation	Room 301BC
THURSDAY	
Company	Convention Center Room
SCIEX	Room 304A
Shimadzu	Room 220
Thermo Fisher Scientific	Room 225CD

MEDIA EVENTS are scheduled for members of the press and financial institutions. All will be held in the Grand Hyatt Hotel.

Company	Monday	Grand Hyatt Hotel Location
Bruker	8:00-9:00 am	Texas Ballroom A
Shimadzu	9:30-10:30 am	Texas Ballroom EF
SCIEX	11:00-12:00 pm	Lone Star Ballroom ABC
Agilent Technologies	1:30-2:30 pm	Lone Star Ballroom DEF
Thermo Fisher Scientific	3:00-4:00 pm	Texas Ballroom D
Waters Corporation	4:30-5:30 pm	Texas Ballroom BC

CONFERENCE REGULATIONS

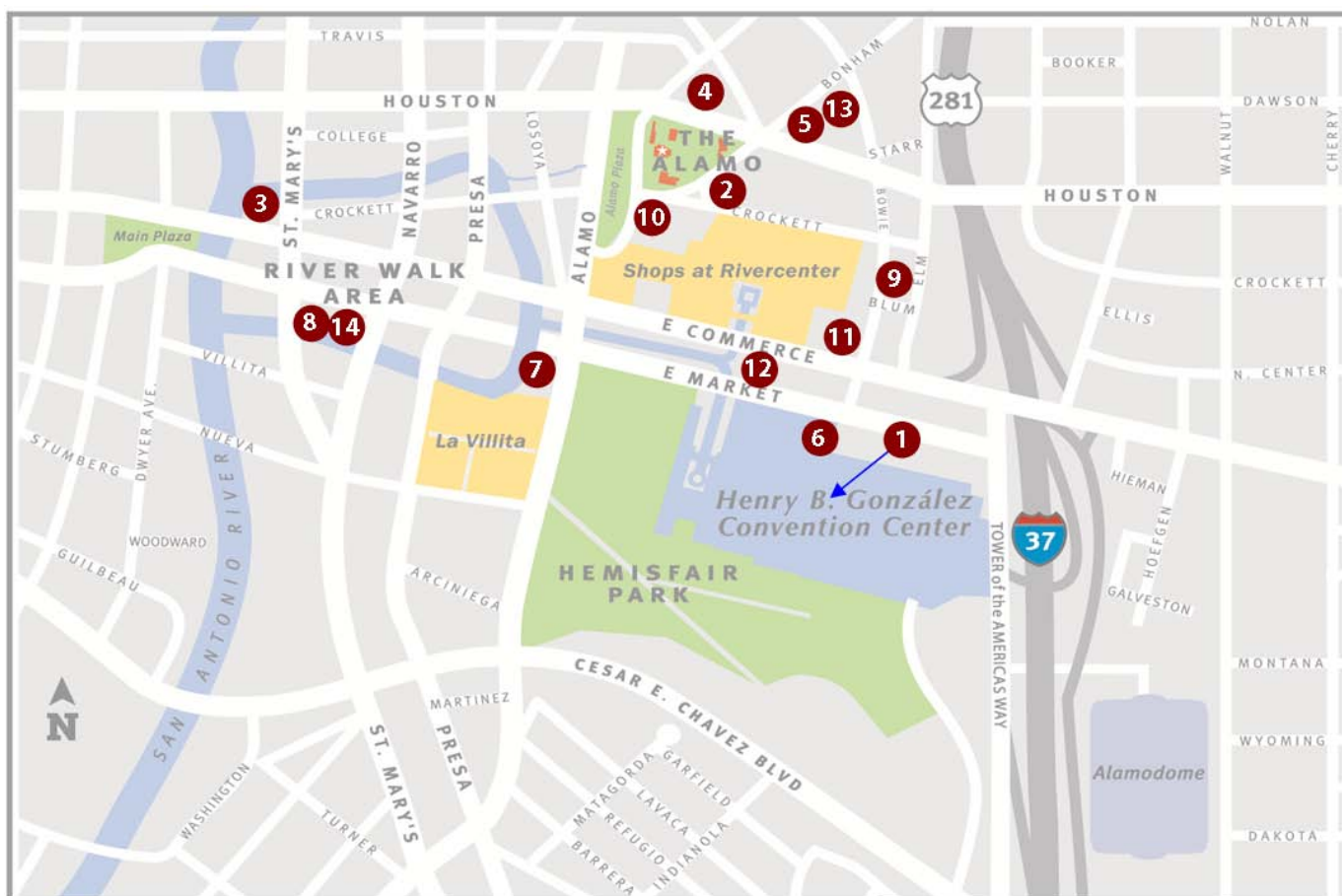
- **Name badge is required** for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- **No smoking** is permitted in the convention center.
- **All devices** must be silenced and screens darkened in oral sessions.
- **No photography** or recording is allowed in oral sessions or in the poster/exhibit Hall.
- **Parents.** Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices for child transport are prohibited in the Poster/Exhibit Hall and hospitality suites.
- **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 express written authority of the author.
- **The placement of advertising** in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.
- **Hardware, accessories or any items for sale** may be displayed only in corporate exhibit booths and hospitality suites.
- **Designated publisher tables** in the conference registration area are for the display of books and journals and must be reserved in advance.
- **There are tables in the registration area for authors** who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.
- **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 hospitality suites** may be used during the daytime hours of 8:00 am – 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.
- **Corporate or institutional logos** on slides or posters may appear only one time in the presentation.

HOTELS



Hotel	Telephone
1. Convention Center	(210) 207-8500
2. Crockett Hotel	(210) 225-6500
3. Drury Inn & Suites Riverwalk	(210) 212-5200
4. Emily Morgan	(210) 225-5100
5. Fairfield Inn & Suites	(210) 212-6262
6. Grand Hyatt San Antonio	(210) 224-1234
7. Hilton Palacio del Rio	(210) 222-1400

Hotel	Telephone
8. Homewood Suites by Hilton	(210) 222-1515
9. La Quinta Inn & Suites	(210) 222-9181
10. Menger Hotel	(210) 223-4361
11. Marriott Rivercenter	(210) 223-1000
12. Marriott Riverwalk	(210) 224-4555
13. Springhill Suites San Antonio	(210) 222-2121
14. Westin Riverwalk	(210) 224-6500





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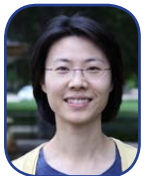
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to these members who were elected to the ASMS Board

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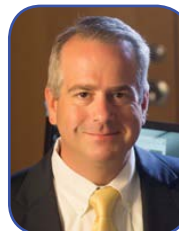
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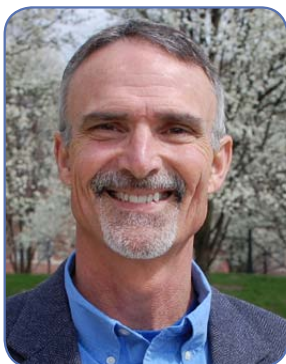


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<i>Ion Mobility MS</i>	Erin Baker Stephen Valentine
<i>Ion Trap MS</i>	Daniel E. Austin Zheng Ouyang
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AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY**2016 RECIPIENT: SCOTT A. MCLUCKEY****AWARD LECTURE: 4:45 PM MONDAY, HALL 1, LEVEL 1**

Dr. Scott A. McLuckey is the recipient of the 2016 ASMS Award for a Distinguished Contribution in Mass Spectrometry for his pioneering contributions to the understanding of the gas-phase ion/ion reactions of polyatomic molecules and their applications in analytical mass spectrometry.

Gas-phase ion chemistry has played a central role in mass spectrometry since its inception. Unimolecular and ion/neutral reactions, for example, have been observed, studied, and used throughout the entire history of molecular mass spectrometry. While the study of ion/ion reactions originated with J.J. Thomson and has been pursued within the context of plasma chemistry, atmospheric chemistry, and chemistry in the interstellar medium, ion/ion reactions have not been exploited in mainstream mass spectrometry until relatively recently. Keys to this development have been the introduction of techniques capable of generating multiply charged ions, electrospray being chief among them, and the use of electrodynamic ion traps, which can store efficiently oppositely charged ions in overlapping time and space. McLuckey and co-workers, beginning at Oak Ridge

National Laboratory in the mid-1990s and continuing at Purdue University since 2000, initiated and sustained a line of research employing electrospray and ion traps that has revealed a wide and expanding array of ion/ion reactions that significantly expand the scope of tandem mass spectrometry, particularly in biological mass spectrometry.

Dr. McLuckey's efforts in this area have focused both on understanding the dynamics of ion/ion reactions and on developing ion/ion reactions for analytical applications. He and his co-workers demonstrated that ion/ion reactions in ion traps can be both highly efficient and fast. Furthermore, ion/ion reactions are universal in that some form of reaction will occur for any combination of oppositely charged ions. Dr. McLuckey's initial work was focused on proton transfer, and to a lesser extent, electron transfer reactions. Proton transfer reactions have been demonstrated to be particularly useful for charge state manipulation and have been used for mixture analysis, concentrating charge, inverting ion charge, etc. Electron transfer has proved to be particularly useful for generating structural information. For example, the discovery in Donald Hunt's lab of reagent anions that transfer electrons to peptide and protein cations led to the development of electron transfer dissociation. These developments, which leveraged much of what was known about proton transfer ion/ion reactions in ion traps, catalyzed the commercial introduction of ion/ion reactions tools that rely on electrospray and ion traps.

In recent years, McLuckey's group has expanded ion/ion chemistry to include selective metal ion insertion/removal and functional group specific covalent bond formation. Collectively, these chemistries, along with proton and electron transfer, significantly expand the power of MS/MS in characterizing peptides, proteins, oligonucleotides and lipids. The wide-ranging efforts of McLuckey and his colleagues in instrumentation, fundamentals, and applications of ion/ion reactions over the past two decades constitute a distinguished contribution to mass spectrometry.

Dr. Scott A. McLuckey is the John A. Leighty Distinguished Professor of Chemistry at Purdue University, West Lafayette, IN.

RON A. HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS**AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3**

The Ron Hites Award recognizes an outstanding publication of original research, based on a paper's innovative aspects, technical and presentation quality, likely stimulation of future research and impact on future applications. The award is named to honor Professor Ron Hites of Indiana University, who led the creation of JASMS in 1988 while president of ASMS. The award includes \$2,000 and a certificate for each author.

The 2016 award recognizes Kevin Pagel, Max Planck Society Berlin, and, co-authors Waldemar Hoffmann and Johanna Hofmann for their paper Energy-Resolved Ion Mobility-Mass Spectrometry: A Concept to Improve the Separation of Isomeric Carbohydrates: JASMS (2014) 25, 471-479.

Left to right Johanna Hofmann, Kevin Pagel, and Waldemar Hoffmann





BIEMANN MEDAL

2016 RECIPIENT: KRISTINA "KICKI" HÅKANSSON

AWARD LECTURE: 4:45 PM TUESDAY, HALL 1, LEVEL 1



Dr. Kristina "Kicki" Håkansson has been awarded the 2016 Biemann Medal for her contributions related to her work to develop and elucidate the mechanisms of electron-based activation methods, including electron capture dissociation, electron detachment dissociation, and electron induced dissociation. She has applied these electron-based activation methods to identify and characterize biological molecules from a number of classes, including peptides, oligonucleotides, and oligosaccharides.

The challenges associated with structural characterization of increasingly complex biological molecules has inspired the development of many new activation methods. Ones involving the attachment or detachment of an electron to an ion have shown great promise and have motivated renewed interest in gas-phase radical ion chemistry, both areas which are hallmarks of the Håkansson group. Dr. Håkansson has focused on deciphering the mechanisms of electron-activated dissociation and shown the outstanding utility of these methods for analysis of nucleic acids, oligosaccharides, and peptides including ones with labile modifications like phosphorylation. Negative ion electron capture dissociation (discovered in the Håkansson laboratory) in particular

has shown excellent performance for characterization of phosphorylated and sulfated peptides ionized in the negative mode. Her group has also shown that electron-activated dissociation methods are gentle enough to allow preservation of higher order structures of nucleic acids.

Dr. Håkansson is a professor in the Department of Chemistry at the University of Michigan in Ann Arbor.

2016 RESEARCH AWARDS

AWARD PRESENTATION: 4:45 PM TUESDAY, HALL 1, LEVEL 1

The Research Awards are fully funded by Thermo Fisher Scientific and Waters Corporation in the amount of \$35,000 each.

Sponsored by

THERMO FISHER SCIENTIFIC



Ronghu Wu
Georgia Institute of
Technology

Sponsored by

WATERS CORPORATION



Etienne Garand
University of Wisconsin-
Madison

2016 POSTDOCTORAL AWARDS**AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3**

Four awards in the amount of \$10,000 each are intended to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities funded by these awards include 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.



John Cahill
Oak Ridge National
Laboratory



Andrew DeBlase
Purdue University



Catherine Going
Stanford University



Pengyuan Liu
The Wistar Institute

2016 STUDENT AWARDS**AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3**

ASMS supports up to ten awards of \$1,000 for graduate students and ten awards of \$500 for undergraduates. Applications and details for these awards are posted to asms.org. The deadline for submission is January 15.

GRADUATE STUDENT AWARDS

Xibei Dang, Florida State University

Zachery Gregorich, University of Wisconsin-Madison

Nathan Hendricks, University of California, Riverside

Johanna Hofman, Max Planck Society

Ramsunder Iyer, University of Tennessee

Brent Kuenzi, University of South Florida

Anumita Saha-Shah, Indiana University

Stephen Sciuto, The University of Toronto

Candice Ulmer, University of Florida

Yeijing Weng, Chinese Academy of Sciences

UNDERGRADUATE STUDENT AWARDS

Willem Duckworth, Clarkson University

Carlo Eikani, Saint Mary's College of California

Matthew Kazaleh, University of Florida

Yekaterina Kori, University of Massachusetts Amherst

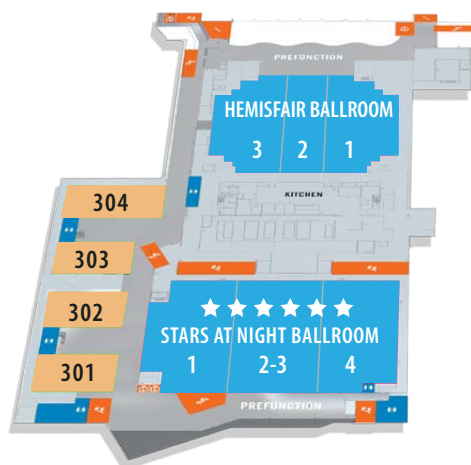
Rebecca Marin, Florida International University

Rachel Martini, University of Michigan

Evan Perez, Duquesne University

LEVEL 3 - BALLROOM LEVEL

- Sessions C (Stars 1)
Session D (Stars 2-3)
Session E (Stars 4)
Session F (Hemisfair 3)
Session G (Hemisfair 2)
Session H (Hemisfair 1)
- Workshops, Breakfast Seminars
(Rooms 301 - 305)



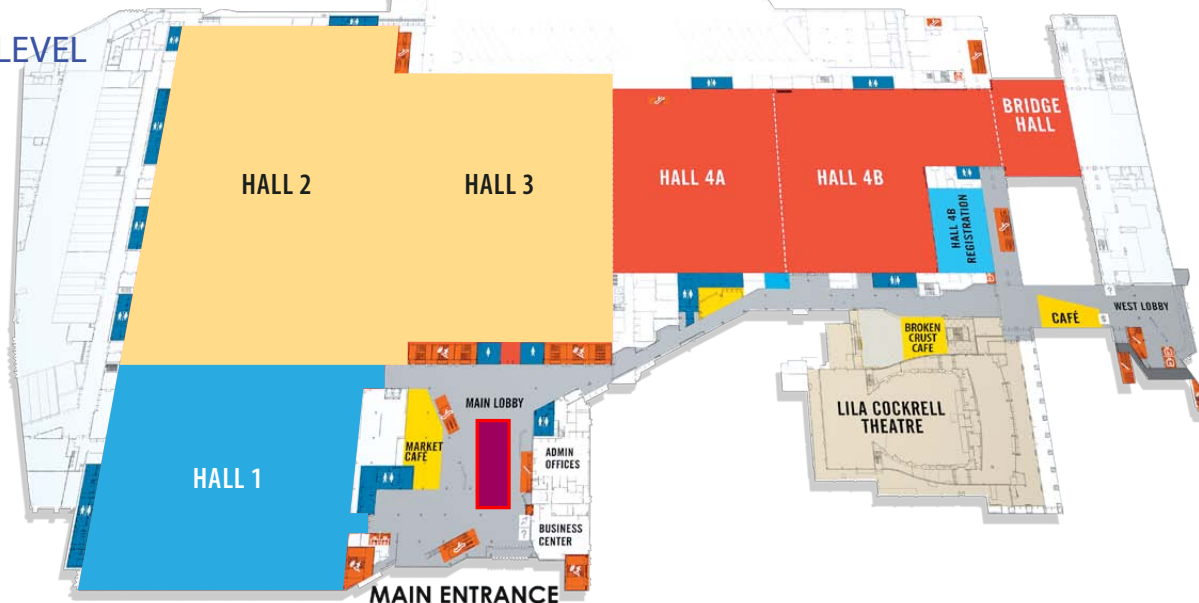
LEVEL 2 - MEETING LEVEL

- Sessions B (Room 221)
- Workshops, Breakfast Seminars
(Rooms 220 - 225)
- Speaker Room (Room 222)



LEVEL 1 - STREET LEVEL

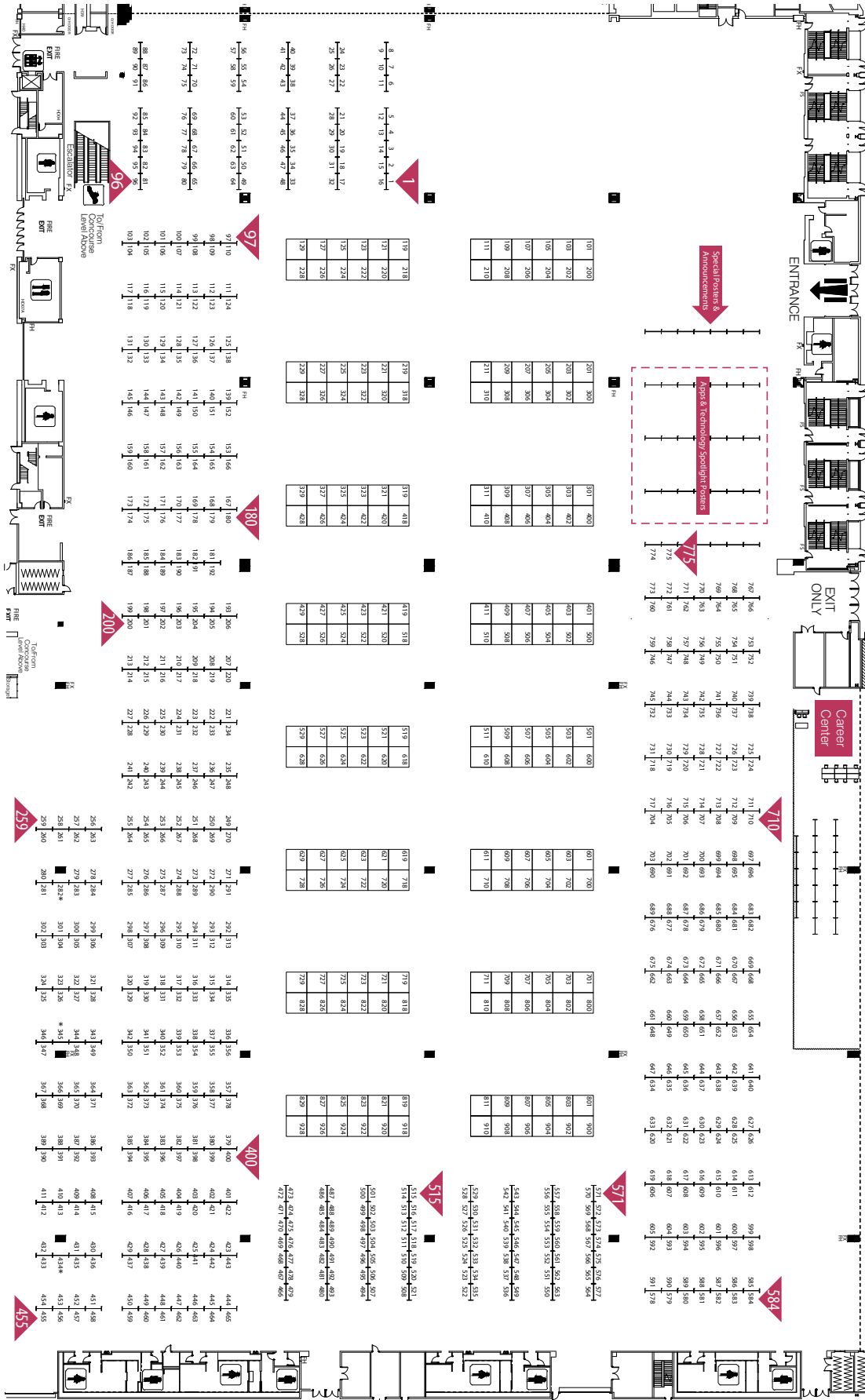
- Posters, Exhibits,
Career Center
(Halls 2 - 3)
- Session A, Plenary
Sessions (Hall 1)
- Registration



Market Street

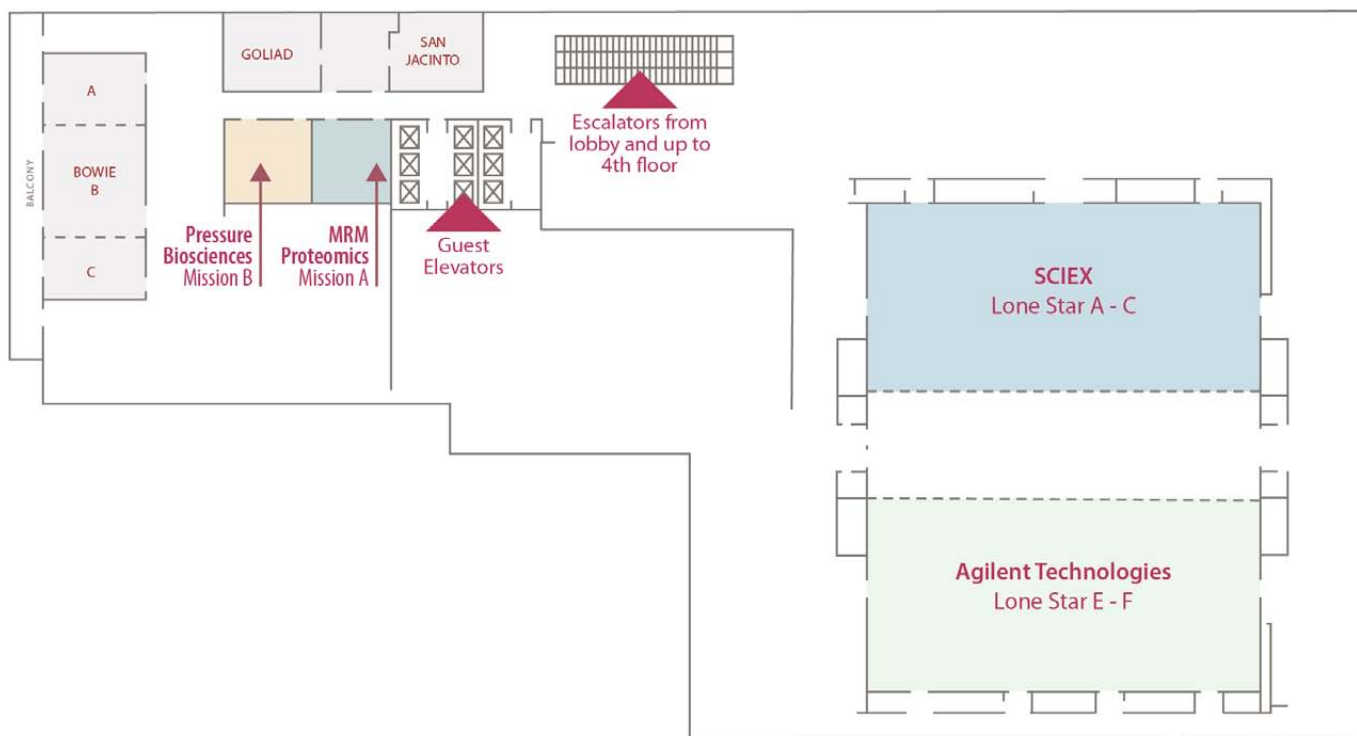
ENTRANCE

EXIT ONLY

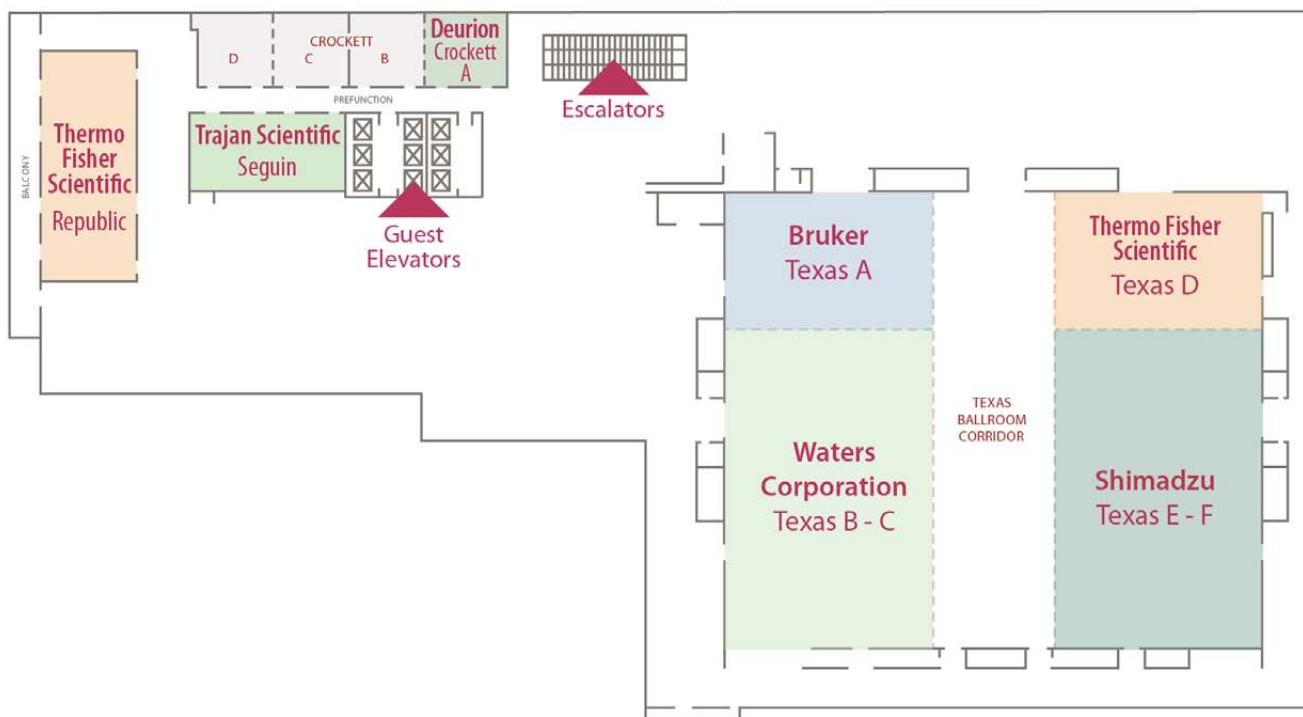




Grand Hyatt, 2nd Floor



Grand Hyatt, 4th Floor



ASMS CORPORATE MEMBERS

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1st Detect		424		
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ACS Publications	Library			
Adeptrix Corporation	Poster	304		
Advanced Chemistry Development (ACD/Labs)	Poster	701		Room 224, Mon (6/6)
Advanced Chromotography		519		
Advanced Energy		219		
Advion Inc.		811		
Agilent Technologies	Poster	200	Lone Star Ballroom DEF	Lone Star Ballroom DEF, Mon-Wed (6/6-6/8)
Alliance Pharma, Inc.		411		
Analytical Parts Supply, LLC		421		
Analytical Sales and Services, Inc.	Poster	107		
Analytical Scientific Instruments		208		
Anasys Instruments		527		
Anest Iwata		703		
Antec		700		
Apricot Designs, Inc.		621		
Ardara Technologies LP		629		
Avanti Polar Lipids, Inc.		427		
BioChromato, Inc.		809		
BIOCRATES Life Sciences AG		121		
Biognosys	Poster	209		
Bioinformatics Solutions Inc.	Poster	318		
Biotage		300		Room 225B, Tue (6/7)
Bonna-Agela Technologies, Inc.	Poster	709		
Bruker Daltonics		329	Texas Ballroom A	Room 225CD, Mon-Wed (6/6-6/8)
Cambridge Isotope Labs		800		
Canadian Life Science	Poster	301		
Cayman Chemical Company		801		
Cerno Bioscience		129		
Chemyx, Inc.		523		
CMP Scientific, Inc.		610		
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Covance		607		
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Denator AB		526		

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Detector Technology, Inc.		500		
Deurion	Poster		Crockett A	
Digital Proteomics	Poster	601		
Drummond Scientific		507		
EBARA Technologies		622		
Edwards Vacuum		504		
Elforlight Ltd.		928		
El-Mul Technologies		810		
e-MSion, Inc.		821		
ESI Source Solutions		328		
ETP Electron Multipliers/Ion Detect		326		
Excellims Corporation		705		
Extrel	Poster	223		
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Genedata		207		
Genetic Engineering & Biotechnology News	Library			
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GenTech Scientific, Inc.		506		
GERSTEL, Inc.	Poster	625		
GL Sciences Inc.		111		Room 301A, Tue (6/7)
Golden West Biologicals, Inc.		202		
Grenova	Poster			
Hamamatsu Corporation	Poster	327		
Hamilton Robotics	Poster	605		
Harris Corp	Poster	711		
HighChem		528		
Horizon Technology, Inc.		628		
HTX Technologies, LLC		829		
HVM Technology		720		
IDEX Health & Science	Poster	400		
iLab Solutions		404		
IMCS		718		
Imtakt USA		211		
Institute for Systems Biology		805		
INTAVIS Bioanalytical Instruments AG		307		
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ionBench		419		
IonSense, Inc.	Poster	119		

ASMS CORPORATE MEMBERS

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ION-TOF GmbH	Poster	518		
IsoSciences		406		
JEOL USA, Inc.		229		
JPT Peptide Technologies		405		
LEAP Technologies		623		
LECO Corporation	Poster	305		Room 303A, Mon-Wed (6/6-6/8)
Linden CMS GmbH		123		
Mac-Mod Analytical		828		
Markes International	Poster	728		
MasCom Technologies		508		
MassTech Inc.		429		
Matrix Science		221		Room 302BC, Mon-Tue (6/6-6/7)
Matsusada Precision Inc.		320		
McKinley Scientific		323		
MeCour Temperature Control		729		
MestreLab Research		502		
Microliter Analytical Supplies (A WHEATON Company)		604		
MilliporeSigma	Poster	721		Room 303BC, Tue (6/7)
Mo Bio Laboratories		222		
Moeller Medical GmbH		524		
MRM Proteomics Inc			Mission A	
MS Noise		529		
mSPEC group		309		
MStm		306		
nanoLiter, LLC	Poster	426		
Nest Group, The	Poster			
New England Peptide, Inc.		227		
New Objective, Inc.	Poster	321		Room 305, Tue-Wed (6/7-6/8)
NIST		308		
Oerlikon Leybold Vacuum		509		
Omni Enclosures		522		
Omni International		511		
OPOTEK, Inc.		606		
Optimize Technologies, Inc.	Poster	608		
Optys Tech Corporation		425		
Owlstone, Inc.		407		
Pall Laboratory		204		
Parker Balston/Hannifin		418		
PEAK Scientific	Poster	619		
Peeke Scientific		624		
Perfinity Biosciences		127		
PerkinElmer		428		

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Phenomenex		226		
Phoenix S&T, Inc.		303		
PHOTONIS	Poster	401		
Physical Electronics	Poster	228		
Phytronix Technologies, Inc.		203		
Presco Incorporated		727		
Pressure BioSciences, Inc.		819	Mission B	
Promega Corporation		618		
Prosolia, Inc.	Poster	423		Room 224, Tue (6/7)
Protea Biosciences, Inc.		325		
Protein Metrics Inc.		510		
Proteome Sciences	Poster			
Proteome Software Inc.		322		
Proton Onsite		105		
PTM Biolabs, Inc.		521		
PurSpec Technologies, Inc.		408		
Pursuits Instrument Limited		803		
Qioptiq, An Excelitas Technologies Co		707		
Rapid Novor Inc.	Poster	206		
Restek Corporation		627		
Resyn Biosciences		704		
RMI Laboratories		224		
Samin Science Co., Ltd		910		
Science/AAAS	Library			
Scientific Instrument Services	Poster	218		
Scientific Systems, Inc.		722		
SCIEX		101	Lone Star Ballroom ABC	Room 302A, Tue-Wed (6/7-6/8) Room 304A, Mon-Thu (6/6-6/9) Room 304BC, Tue-Wed (6/7-6/8) Room 305, Mon (6/6)
Shimadzu Scientific Instruments, Inc.	Poster	210	Texas Ballroom EF	Room 220, Mon-Thu (6/6-6/9)
Shimifrez Inc.		708		
Sierra Analytics		422		
Silantes GmbH		603		
Sound Analytics		702		
Spark Holland		525		
SpectralWorks Limited	Poster	205		
Spectroscopy		402		
Spectroswiss		311		
Spellman High Voltage		620		

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SYFT Technologies	Poster	609		
Tecan	Poster	220		
The Analytical Scientist	Library			
Thermo Fisher Scientific		319	Texas Ballroom D and Republic ABC	Room 225CD, Thu (6/9) Republic ABC, Mon-Wed (6/6-6/8)
Tofwerk AG		225		
Tosoh Bioscience		324		
Trajan Scientific and Medical	Poster	403	Seguin AB	
Veritomyx		818		
VICI Valco Instruments		109		
VRS		103		
VUV Analytics		900		
Waters Corporation	Poster	201	Texas Ballroom BC	Room 301A, Mon (6/6) Room 301BC, Mon-Wed (6/6-6/8) Texas Ballroom BC, Mon-Wed (6/6-6/8)
Wiley	Library			
XPC Corporation		302		
Zef Scientific Inc.		602		
Zhejiang Haochuang Biotech Co., Ltd	Poster	826		

PROGRAM ACKNOWLEDGEMENTS

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Vicki H. Wysocki
The Ohio State University
Vice President for Programs

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

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PROGRAM OVERVIEW

SATURDAY

9:00 AM - 4:30 PM	SHORT COURSES
1:00 - 5:00 PM	REGISTRATION

SUNDAY

9:00 AM - 4:30 PM	SHORT COURSES
10:00 AM - 8:00 PM	REGISTRATION
4:00 - 4:45 PM	ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS, Stars Ballroom 1, level 3
5:00 - 6:30 PM	TUTORIAL LECTURES, Hall 1, level 1 <div>  <p>5:00 - 5:45 pm Forensic Mass Spectrometry #TellMeSomethingIDontKnow Facundo Fernandez Georgia Institute of Technology</p> </div> <div>  <p>Glen Jackson West Virginia University</p> </div> <div>  <p>5:45 - 6:30 pm An Analyte's Journey from Solution into the Gas Phase Lars Konermann University of Western Ontario</p> </div>
6:45 - 7:45 PM	CONFERENCE OPENING, Hall 1, level 1 Vicki Wysocki (The Ohio State University), ASMS Vice President for Programs <div>  <p>A Molecular Arsenal Against Ebola Virus Erica Ollmann Saphire The Scripps Institute-La Jolla</p> </div>
7:45 - 9:00 PM	WELCOME RECEPTION IN THE POSTER/EXHIBIT HALL Undergraduate Student Poster Competition


PROGRAM OVERVIEW

MONDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS <ul style="list-style-type: none"> MOAam: Synthetic Polymers, Hall 1, level 1 MOBam: Fundamentals: Ion-Ion and Ion-Neutral Interactions, Room 221, level 2 MOCam: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, Stars Ballroom 1, level 3 MODam: Instrumentation: FTMS, Stars Ballroom 2-3, level 3 MOEam: Diagnostic Clinical Chemistry, Stars Ballroom 4, level 3 MOFam: Informatics: Discovery Proteomics, Hemisfair Ballroom 3, level 3 MOGam: Metabolomics: Untargeted Profiling, Hemisfair Ballroom 2, level 3 MOHam: Membrane Protein MS, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Monday Posters, Poster/Exhibit Hall, level 1 Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm. 11:30 – 1:00 pm: Undergraduate students – look for reserved tables and free lunch vouchers to <i>Meet the Experts</i>
2:30 - 4:30 PM	ORAL SESSIONS <ul style="list-style-type: none"> MOApm: Food Safety and Chemistry: Foodomics, Allergens, Bacteria, Foods, Hall 1, level 1 MOBpm: Fundamentals: Ion Spectroscopy, Room 221, level 2 MOCpm: Instrumentation: New Developments in Ionization and Sampling, Stars Ballroom 1, level 3 MODpm: Antibodies and Antibody Drug Conjugates, Stars Ballroom 2-3, level 3 MOEpm: Data Independent Acquisition: Innovative Methods and Applications, Stars Ballroom 4, level 3 MOFpm: Informatics: Metabolomics, Hemisfair Ballroom 3, level 3 MOGpm: Nucleic Acid MS, Hemisfair Ballroom 2, level 3 MOHpm: Covalent Labeling and Chemical Crosslinking, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	AWARD LECTURE , Hall 1, level 1 Award for a Distinguished Contribution in Mass Spectrometry  Scott A. McLuckey Purdue University
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas. 01 Top-Down Proteomics: Ready for Primetime? Room 220, level 2 02 Next Generation LC-MS: Critical Insights & Future Perspectives, Room 221, level 2 03 Art and Cultural Heritage Mass Spec Applications, Room 225A, level 2 04 Bioinformatics: Challenges & Opportunities in Proteogenomics (Bioinformatics for MS), Room 225B, level 2 05 Environmental Analysis: Emerging Topics (Environmental Applications Interest Group), Room 225C, level 2 06 Metal Cationization in MS/MS of Biomolecules (Metal Ion Coordination Chemistry Interest Group), Room 225D, level 2 07 Proteomics Informatics for the Trans-Proteomic Pipeline, Room 301A, level 3 08 Metabolomics: Emerging Technologies for Continued Innovation (Metabolomics Interest Group), Room 301BC, level 3 09 Polymer MS Technology: Advancements and Discussion (Polymeric Materials Interest Group), Room 302A, level 3 10 MS Analysis of Antibody-Drug Conjugates (Pharmaceuticals Interest Group), Room 302BC 11 Protocol Repositories for Proteomics and Metabolomics (Analytical Lab Managers Interest Group), Room 303A, level 3 12 Miniaturization of Ion Traps and Related Devices (Ion Trap Interest Group), Room 303BC 13 MS Career Options: How to Kick-Start your Career (Young Mass Spectroscopists Interest Group), Room 304, level 3 14 System Performance: Tracking through Statistical QC Monitoring (LC/MS & Related Topics Interest Group), Room 305, level 3
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Grand Hyatt Hotel

PROGRAM OVERVIEW

TUESDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS <ul style="list-style-type: none"> • TOAam: Energy, Petroleum, and Biofuels: Instrumentation and Method Development, Hall 1, level 1 • TOBam: Fundamentals: Metal Ion Cationization, Metal-Ligand Interactions and Catalysis, Room 221, level 2 • TOCam: HRMS for Quantitation in Drug Discovery, Development and Beyond, Stars Ballroom 1, level 3 • TODam: Imaging: Instrumentation & Method Development, Stars Ballroom 2-3, level 3 • TOEam: Quantitative Proteomics in Systems Biology, Stars Ballroom 4, level 3 • TOFam: Instrumentation: non-FT based Analyzers, Hemisfair Ballroom 3, level 3 • TOGam: Lipids and Profiling, Hemisfair Ballroom 2, level 3 • TOHam: Native MS in Structural Biology, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Tuesday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	ORAL SESSIONS <ul style="list-style-type: none"> • TOApm: Environmental: New Instrumentation and Approaches, Hall 1, level 1 • TOBpm: New Developments in Ion Detection, Room 221, level 2 • TOCpm: Quantitative Analysis in Drug Discovery and Development, Stars Ballroom 1, level 3 • TODpm: Ion Mobility, FAIMS & DMS: New Developments & Applications, Stars Ballroom 2-3 • TOEpm: Qualitative and Quantitative Analysis of Post-translational Modifications, Stars Ballroom 4, level 3 • TOFpm: Imaging: Computational Methods and Analysis, Hemisfair Ballroom 3, level 3 • TOGpm: Metabolomics: New Technologies and Applications, Hemisfair Ballroom 2, level 3 • TOHpm: Protein-Ligand Interactions, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	AWARD LECTURE , Hall 1, level 1  Kristina "Kicki" Håkansson University of Michigan
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas <ol style="list-style-type: none"> 01 Glycoproteomics: Site Specific Glycan Analysis, Room 220, level 2 02 Ion Mobility: How to Interpret the Data (Ion Mobility MS Interest Group), Room 221, level 2 03 H/D Exchange, Covalent Labeling & Cross-Linking (H/D Exchange, Covalent Labeling & Cross-Linking Interest Group), Room 225A, level 2 04 Food Safety & Security: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group), Room 225B, level 2 05 Microcontrollers and Microcomputers: Emerging Technologies, Room 225C, level 2 06 DNA/RNA Adducts: Assay Development in Detection and Quantification (Oligonucleotides and Nucleic Acids Interest Group), Room 225D, level 2 07 Petroleum and Biofuels: Handling the Data (Energy, Petroleum & Biofuels Interest Group), Room 301A, level 3 08 Metabolism of Biotherapeutics: When, Why and How? (DMPK Interest Group), Room 301BC, level 3 09 Modification of Commercial Instruments for Fundamental Research (Fundamentals Interest Group), Room 302A, level 3 10 Lipidomics in the Era of Systems Biology: The Big Fat Challenges (Lipids and Lipidomics Interest Group), Room 302BC, level 3 11 Undergraduate Research in Mass Spectrometry (Undergraduate Research in MS Interest Group), Room 303A, level 3 12 The Chorus Project: Sustainable Cloud Solution for MS Data, Room 303BC, level 3 13 Data Independent Acquisition (Data Independent Acquisition Interest Group), Room 304, level 3 14 Good Manufacturing Practice (GMP); Mass Spectrometric Instrument Qualification, Room 305
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Grand Hyatt Hotel

PROGRAM OVERVIEW

WEDNESDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS <ul style="list-style-type: none"> WOAam: Energy, Petroleum and Biofuels: Structure, Quantification, and Data Analysis, Hall 1 level 1 WOBam: Fundamentals: Energetics and Mechanisms of Uni and Bimolecular Reactions, Room 221, level 2 WOCam: Imaging: Pharmaceuticals and Metabolites, Stars Ballroom 1, level 3 WODam: Instrumentation: Miniaturization of MS, Stars Ballroom 2-3, level 3 WOEam: Biomarkers: Qualitative Analysis, Stars Ballroom 4, level 3 WOFam: Informatics: Multiomics Integration and Application, Hemisfair Ballroom 3, level 3 WOGam: MS in the QC Lab, Hemisfair Ballroom 2, level 3 WOHam: Macromolecular Complexes, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Wednesday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	ORAL SESSIONS <ul style="list-style-type: none"> WOApm: Exposomics: Targeted, Untargeted and Bioinformatics Methodologies, Hall 1, level 1 WOBpm: Fundamentals: Molecular Modeling and Quantum Mechanical Calculations in IM and MS, Room 221, level 2 WOCpm: Environmental: Emerging Contaminants, Stars Ballroom 1, level 3 WODpm: Imaging: Biomedical Applications, Stars Ballroom 2-3, level 3 WOEpm: Top Down Protein Analysis, Stars Ballroom 4, level 3 WOFpm: MS in the Regulatory Environment, Hemisfair Ballroom 3, level 3 WOGpm: Carbohydrates, Hemisfair Ballroom 2, level 3 WOHpm: New Separations Approaches Coupled to MS, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	ASMS MEETING , Stars Ballroom 1, level 3: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas. <ol style="list-style-type: none"> 01 Bioanalysis: Current Status of Strategy and Practice of a Tiered Approach (Regulated Bioanalysis Interest Group), Room 220, level 2 02 Large-Scale Analysis of MS Big Data: From Data to Knowledge and Back, Room 221, level 2 03 FTMS: Day-to-Day Concerns for High Resolution Mass Analysis (FTMS Interest Group), Room 225A, level 2 04 Novel Mass Spectrometry Instrumentation: Moving into the Hands of Practitioners (Forensics & Homeland Security Interest Group), Room 225B, level 2 05 Photoionization: New Developments (Photoionization MS Interest Group), Room 225C, level 2 06 The NIH Review and Funding Process, Room 225D, level 2 07 Entrepreneurship: Creating a Job in Mass Spectrometry, Room 301A, level 3 08 Protein Quantitation (Absolute) by LC-MS: Biomarker and Biotherapeutic, Room 301BC, level 3 09 Isomeric Glycans: Characterization & Quantitation, Room 302A, level 3 10 Protein Therapeutics: Characterization using MS (Biotherapeutics Interest Group), Room 302BC, level 3 11 The Exposome: MS-based Metabolomic Workflows to Characterize the Exposome (Exposomics Interest Group), Room 303A, level 3 12 Biomarker Translation: Quality Control & Quality Assurance (Clinical Chemistry Interest Group), Room 303BC, level 3 13 Imaging MS: Present and Future of Multimodal Studies (Imaging MS Interest Group), Room 304, level 3 14 Galaxy for Proteomics Data Analysis: An Interactive Demonstration, Room 305, level 3
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , Grand Hyatt Hotel



PROGRAM OVERVIEW

THURSDAY

7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS <ul style="list-style-type: none"> • ThOAam: New Concepts for Forensic MS, Hall 1, level 1 • ThOBam: Fundamentals: Photodissociation, Room 221, level 2 • ThOCam: New Developments in Ionization and Sampling for DMPK, Stars Ballroom 1, level 3 • ThODam: Translational Success with MS, Stars Ballroom 2-3, level 3 • ThOEam: Glycopeptides and Glycoproteins, Stars Ballroom 4, level 3 • ThOFam: Informatics: Targeted Proteomics and DIA, Hemisfair Ballroom 3, level 3 • ThOGam: Application of Stable Isotope Labeling in MS, Hemisfair Ballroom 2, level 3 • ThOHam: Ion Mobility: Structure, Hemisfair Ballroom 1, level 3
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Thursday Posters, Poster/Exhibit Hall Odd-number posters present 10:30 am - 1:00 pm. Even-number posters present 12:00 - 2:30 pm.
2:30 - 4:30 PM	ORAL SESSIONS <ul style="list-style-type: none"> • ThOApm: Food Safety and Chemistry: Non-targeted Screening, Hall 1, level 1 • ThOBpm: Fundamentals: Ion Activation and Dissociation, Room 221, level 2 • ThOCpm: MS Solutions for Drug Metabolism Challenges, Stars Ballroom 1, level 3 • ThODpm: Ambient Ionization: Instrumentation & Applications, Stars Ballroom 2-3, level 3 • ThOEpm: Biomarkers: Quantitative Analysis, Stars Ballroom 4, level 3 • ThOFpm: Informatics: Peptide and Protein Identification, Hemisfair Ballroom 3, level 3 • ThOGpm: Lipidomics: New MS Technologies and Applications, Hemisfair Ballroom 2, level 3 • ThOHpm: Hydrogen-Deuterium Exchange MS, Hemisfair Ballroom 1, level 3
4:45 - 5:30 PM	PLENARY LECTURE , Hall 1, level 1 <div data-bbox="375 945 553 1192" data-label="Image"> </div> <div data-bbox="587 989 1256 1050" data-label="Text"> <p>More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds</p> </div> <div data-bbox="587 1075 812 1134" data-label="Text"> <p>William Bialek Princeton University</p> </div>
6:30 - 9:00 PM	CLOSING EVENT Briscoe Western Art Museum. Ticket required

SUNDAY EVENING, 4:00 - 9:00 PM

4:00 – 4:45 PM, SUNDAY
Attention First-time Graduate Students and Undergrads
Plan your Strategy: What to See and Do at ASMS
 Elaine Marluff and JC Poutsma, presiding
 Stars Ballroom 1, level 3

5:00 – 6:30 PM, SUNDAY
TUTORIAL SESSION
 Vicki Wysocki (The Ohio State University) presiding
 Hall 1, level 1



5:00 – 5:45 pm
Forensic Mass Spectrometry
#TellMeSomethingIDontKnow

Facundo Fernandez
 Georgia Institute of Technology



Glen Jackson
 West Virginia University



5:45 – 6:30 pm
An Analyte's Journey from Solution into the Gas Phase

Lars Konermann
 University of Western Ontario

6:45 – 7:45 PM, SUNDAY
CONFERENCE OPENING
 Vicki Wysocki (The Ohio State University) presiding
 Hall 1, level 1

Welcome, Vicki H. Wysocki (The Ohio State University)
 ASMS Vice President for Programs



A Molecular Arsenal Against Ebola Virus

Erica Ollmann Saphire
 The Scripps Institute-La Jolla

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

MONDAY MORNING ORAL SESSIONS

8:30-10:30 am MONDAY
SYNTHETIC POLYMERS
 Paul Kowalski (Bruker Daltonics, Inc.)
 Hall 1, level 1

- MOA am 08:30 **Mechanistic Studies of Hafnocene Catalyzed Olefin Polymerization;** Anthony Paul Gies¹; Roger Kuhlman²; Cristiano Zuccaccia³; Alceo Macchioni³; ¹Dow Chemical Company, Freeport, TX; ²Univation Technologies, Freeport, TX; ³Dipartimento di Chimica, Biologia e Biotecnologie and CIRCC, University of Perugia, Perugia, Italy
- MOA am 08:50 **Analytical Characterization of PEG and PEG conjugates by Mass Spectrometry;** Guanghui Han¹; Wilson Phung¹; Whitney Shatz¹; Julie Q. Hang¹; Justin Scheer¹; Paul Schnier¹; Wendy Sandoval¹; ¹Genentech Inc, South San Francisco, CA
- MOA am 09:10 **The Use of Iodo-functionalized Polydisperse Polymers as Mass-defect Tuned Calibrants;** Joseph A. Giesen¹; Jennifer L. Marple¹; Scott M. Grayson¹; ¹Tulane University, New Orleans, LA
- MOA am 09:30 **Sequence and Conformational Analysis of Recombinant Polypeptide-Polymer Conjugates;** Sahar Sallam¹; Bradford A Paik²; Xinqiao Jia²; Chrys Wesdemiotis¹; ¹The University of Akron, Akron, OH; ²University of Delaware, Newark, DE
- MOA am 09:50 **Using MS/MS to Design Information-Encoded Synthetic Copolymers;** Laurence Charles¹; Jean-François Lutz²; ¹Aix-Marseille University, Marseille

Cedex 20, PACA; ²Institut Charles Sadron, Strasbourg, France

MOA am 10:10 **Peptoid Fragmentation -The Bias toward Y-Ion Formation;** Jianhua Ren¹; Yuan Tian²; Ekram Hossain²; Michael Connolly³; Ronald Zuckermann³; ¹University of the Pacific, Stockton, CA; ²University of the Pacific, Stockton, CA; ³Lawrence Berkeley National Laboratory, Berkeley, CA

8:30-10:30 am MONDAY
FUNDAMENTALS: ION-ION AND ION-NEUTRAL INTERACTIONS
 John E. P. Syka (Thermo Fisher Scientific)
 Room 221, level 2

- MOB am 08:30 **Preparation of a Dianion with the Highest Known Proton Affinity: Ortho-Diethynyl Benzene;** Berwyck Poad¹; Nicholas Reed²; Christopher Hansen²; Adam Trevitt²; Stephen J Blanksby¹; Emily Mackay³; Michael Sherburn³; Bun Chan⁴; Leo Radom⁴; ¹Queensland University of Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia; ³Australian National University, Canberra, Australia; ⁴The University of Sydney, Sydney, Australia
- MOB am 08:50 **Evaluating Gas-Phase Folding of Protein Ions Using Cation to Anion Proton Transfer;** Kenneth J. Laszlo¹; Eleanor B. Munger¹; Stephanie C. Heard²; Matthew F Bush¹; ¹University of Washington, Seattle, WA; ²Kalamazoo College, Kalamazoo, MI

- MOB am 09:10 **Selective Oxidation via Ion/Ion Reactions: Characteristic Chemistries for Methionine Residues and Cysteine Post-Translational Modifications**; Alice Pilo¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MOB am 09:30 **Identification of Carboxylic Acids in Protonated Drug Metabolites by using Ion-molecule Reactions in a Linear Quadrupole Ion Trap Mass Spectrometer**; Joann Max¹; Xin Ma²; Rashmi Kumar³; Hilka I Kenttamaa³; ¹Purdue University, West Lafayette, IN; ²Purdue University-Department of Chemistry, West Lafayette, IN; ³West Lafayette, IN
- MOB am 09:50 **Ultraviolet Photodissociation of Native Proteins Following Proton Transfer Reaction in an Orbitrap Elite Mass Spectrometer**; Dustin D Holden; Jennifer Brodbelt¹; ¹The University of Texas, Austin, TX
- MOB am 10:10 **High-throughput Proteomics with Negative Electron Transfer Dissociation (NETD)**; Nicholas Riley¹; Michael S Westphall¹; Joshua J Coon¹; ¹University of Wisconsin-Madison, Madison, WI

**8:30-10:30 am MONDAY
ION MOBILITY: SMALL MOLECULES,
PHARMACEUTICALS, AND DMPK
Cris Laphorn (University of Greenwich)
Stars Ballroom 1, level 3**

- MOC am 08:30 **Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications**; John Fjeldsted¹; Ruwan T Kurulugama¹; Alex Mordehai¹; Emma E Rennie¹; Ed Darland¹; George C Stafford¹; Jody May²; Sarah M Stow²; John A McLean²; Tim Causon³; Teresa Mairinger³; Stephan Hann³; Erin Baker⁴; ¹Agilent Technologies, Santa Clara, CA; ²Vanderbilt University, Nashville, TN; ³Universität für Bodenkultur, Vienna, Austria; ⁴Pacific Northwest National Lab, Richland, WA
- MOC am 08:50 **Stereoisomer Separation by Ion Mobility – Mass Spectrometry of Multivalent Cation-Chiral Small Molecule Complexes**; Christopher Chouinard¹; Robin HJ Kemperman¹; Nicholas M Oranzi¹; Harrison M King¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL
- MOC am 09:10 **High-throughput Screening Strategy for Tracking Synthetic Biology Variants Libraries using Robotic Platforms and Colormetric Assays Combined with Fast LC-IM MS**; Cunyu Yan¹; Mark Dunstan²; Nicholas Rattray²; Perdita Barran²; ¹University of Manchester, Manchester, Manchester; ²University of Manchester, Manchester, UK
- MOC am 09:30 **Amino Acid Separation using Different Drift Gases in an RF-Confining Drift Cell**; Kimberly Davidson¹; Matthew F Bush¹; ¹University of Washington, Seattle, WA
- MOC am 09:50 **Structural Characterization of Monomers and Oligomers of D-Amino Acid Containing Peptides using Linear and Nonlinear Ion Mobility Separations**; Xueqin Pang¹; Chenxi Jia¹; Matthew Baird²; Zhengwei Chen³; Alexandre A Shvartsburg²; Lingjun Li^{1,3}; ¹School of Pharmacy, University of Wisconsin Madison, WI; ²Wichita State University, Wichita, KS; ³Department of Chemistry, UW-Madison, WI
- MOC am 10:10 **Preparative Ion Mobility Spectrometry using an Inline Periodic Focusing Differential Mobility Analyzer (PFDMA)**; Kent Gillig¹; Chung-Hsuan Chen²; ¹Academia Sinica, Taipei, Nankang, Section 2, Taipei 115; ²Academia Sinica, Genomics Research Center Taipei, Taiwan

**8:30-10:30 am MONDAY
INSTRUMENTATION: FTMS
Hilka Kenttamaa (Purdue University)
Stars Ballroom 2-3, level 3**

- MOD am 08:30 **New Gated Approach for Coupling Trapped Ion Mobility Spectrometry to Fourier Transform Ion Cyclotron Mass Spectrometry**; Mark Ridgeway¹; William Danielson²; Jeremy Wolf¹; Melvin Park¹; ¹Bruker Daltonic, Billerica, MA; ²Danielson Software Consulting, Richland, WA
- MOD am 08:50 **Multi-CRAFTI: Simultaneous Measurement of Relative Collision Cross Sections for Multiple Ions Measured using Fourier Transform Ion Cyclotron Resonance Linewidths**; David V. Dearden¹; Anupriya Anupriya¹; ¹Brigham Young University, Provo, UT
- MOD am 09:10 **21 Tesla FT-ICR Mass Spectrometer for Ultrahigh Resolution Analysis of Complex Mixtures**; Donald F. Smith¹; David C. Podgorski^{1,2}; Yuri E Corilo^{1,2}; Christopher L. Hendrickson¹; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, FSU Tallahassee, FL
- MOD am 09:30 **Surface Induced Dissociation (SID) of Protein Complexes in a Hybrid FT-ICR**; Jing Yan¹; Mowei Zhou²; Gilbert Joshua¹; Jeremy J. Wolff³; Randall E. Pedder⁴; Arpad Somogyi⁵; Royston S. Quintyn¹; Lindsay Morrison¹; Michael L. Easterling³; Ljiljana Pasa-Tolic²; Vicki H. Wysocki¹; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ³Bruker Corporation, Billerica, MA; ⁴Ardara Technologies L.P., Ardara, PA; ⁵OSU Mass Spectrometry & Proteomics Facility, The Ohio State University, Columbus, OH
- MOD am 09:50 **Construction of a Dual-Detector Fourier Transform Electrostatic Linear Ion Trap Utilizing In-Trap Potential Lift**; Eric Dziekonski¹; Robert Santini¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MOD am 10:10 **Influence of Ion Clouds Micromotion on FTICR Mass-Spectrometer Performances in Ultrahigh Resolution Mode of Operation**; Eugene Nikolaev¹; Gleb Vladimirov^{2,1}; Goekhan Baykut³; Roland Jertz³; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russia; ²Skolkovo Institute of Technology, Moscow, Russia; ³Bruker Daltonic GmbH, Bremen, Germany

**8:30-10:30 am MONDAY
DIAGNOSTIC CLINICAL CHEMISTRY
Heather C. Kuiper (CDC)
Stars Ballroom 4, level 3**

- MOE am 08:30 **Intraoperative Diagnosis of Gliomas using Desorption Electrospray Ionization Mass Spectrometry: A Review of Clinical Cases**; Valentina Pirro¹; Alan K. Jarmusch²; Zane R. Baird²; Clint Alfaro³; Eyas Hattab³; Aaron Cohen-Gadol³; Graham R Cooks²; ¹Purdue University, West Lafayette, Indiana; ²Purdue University, West Lafayette, IN; ³Indiana University School of Medicine, Indianapolis, IN
- MOE am 08:50 **DESI-MSI-based Diagnostics of Cirrhotic Liver Diseases**; Anna Mroz¹; Francesca Rosini¹; Alex Pechlivanis¹; Luisa Doria¹; Evaggelia Liaskou²; Gideon Hirschfield²; Simon Taylor-Robinson¹; David Jones³; Robert Goldin¹; Elaine Holmes¹; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom



- MOE am 09:10 Kingdom; ²University of Birmingham, Birmingham, UK; ³Newcastle University, Newcastle upon Tyne, UK
On-demand Disease Diagnosis using 3D Microfluidic Paper-based Analytical Devices Capable of On-chip Mass Spectrometry; Abraham Kwame Badu Tawiah¹; Suming Chen¹; Deidre E Damon¹; ¹Ohio State University, Columbus, OH
- MOE am 09:30 **Clinical Diagnosis of Botulism with Mass Spectrometry;** Suzanne R. Kalb¹; Dongxia Wang¹; Jakub Baudys¹; Kaitlin Hoyt²; Kathryn Pigg²; John R Barr¹; ¹CDC, Atlanta, GA; ²Battelle Memorial Institute, Atlanta, GA
- MOE am 09:50 **Typing of Bacterial Strains using Ultrahigh Resolution MALDI-FTICR-MS;** Frank Fleurbaaij¹; Margriet E.M. Kraakman²; Eric C. J. Claas²; Wilco C. Knetsch²; Hans C. van Leeuwen²; Yuri E.M. van der Burgt¹; Karin Ellen Veldkamp²; Wil Goessens³; Bart J. Mertens⁴; Ed J. Kuijper²; Paul J. Hensbergen¹; Simone Nicolardi¹; ¹Center for Proteomics and Metabolomics, LUMC, Leiden, NL; ²Department of Medical Microbiology, LUMC, Leiden, NL; ³Department of Medical Microbiology and Infectious Disease, Erasmus MC, Rotterdam, NL; ⁴Department of Medical Statistics, LUMC, Leiden, NL
- MOE am 10:10 **The Necessity for Liquid Chromatography in Drug of Abuse Analysis for Resolution of Opiate-Derived Interferences;** Brian Rappold; *Essential Testing, Collinsville, IL*

**8:30-10:30 am MONDAY
INFORMATICS: DISCOVERY PROTEOMICS**

**Xiaowen Liu (Indiana University)
Hemisfair Ballroom 3, level 3**

- MOF am 08:30 **Enabling Massive Blind Database Search using Multiple Enzyme Proteomics;** Laurence E. Bernstein¹; Seungjin Na¹; Nuno Bandeira^{2,3,4}; ¹University of California San Diego, San Diego, CA; ²Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; ³Computer Science and Engineering, University of California San Diego, La Jolla, CA; ⁴Skaggs School of Pharmacy, UC San Diego, La Jolla, CA
- MOF am 08:50 **Embracing Complexity and Diversity: Discovery Metaproteomics of Multiple Microbiomes using the Galaxy Framework;** Pratik Jagtap¹; Brian Sandri²; Somaieh Afiuni-Zadeh²; Kevin Viken²; Kristin Boylan²; Jim Johnson³; Thomas F McGowan³; Maneesh Bhargava²; Chris Wendt²; Amy Skubitz²; Joel Rudney²; Tim Griffin²; ¹Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN; ²University of Minnesota, Minneapolis, MN; ³University of Minnesota Supercomputing Institute, Minneapolis, MN
- MOF am 09:10 **Maximizing Shotgun Proteomics Isobaric Tagging Data Output using MS/MS Multi-Objective Optimization Algorithm;** John Corthésy¹; Kostantinos Theofilatos²; Seferina Mavroudis^{2,3}; Ornella Cominetti¹; Mona Remlawi⁴; Francesco Ferraro⁴; Antonio Núñez Galindo¹; Ivan Montoliu¹; Martin Kussmann¹; Spiros Likothanassis^{2,5}; Loïc Dayon¹; ¹Molecular Biomarkers Core, Nestlé Institute of Health Sciences, Lausanne, Switzerland; ²InSybio Ltd., London, United Kingdom; ³Department of Social Work, School of Sciences of Health and Care, Technological Educational Institute of Patras, Patras, Greece; ⁴Bio System Informatics, Nestlé Institute of Health Sciences, Lausanne, Switzerland; ⁵Department of Computer Engineering and Informatics of the University of Patras, Patras, Greece

- MOF am 09:30 **Real-Time Informatics: A Database Search Increases Depth and Accuracy of Isobaric Label Quantitation in Discovery Proteomics;** Christopher Michael Rose¹; Derek J Bailey²; Joao Paulo¹; Jeremy D O'Connell¹; David P Nusinow¹; Joel M Chick¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA; ²Thermo Fisher Scientific, San Jose, CA
- MOF am 09:50 **An informatic Framework for Defining Multi-Proteoform Complexes (MPCs) by Native Top-Down Mass Spectrometry;** Nicole A Haverland¹; Owen S Skinner¹; Pierre C Havugimana¹; Luca Fornelli¹; Bryan P Early¹; Joseph B Greer¹; Ryan T Fellers¹; Kenneth R Durbin¹; Luis H. F. Do Vale²; Rafael D Melani¹; Henrique S Seckler¹; Micah Nelp³; Richard D LeDuc¹; Vahe Bandarian³; Philip D. Compton¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²University of Brasilia, Brasilia, Brazil; ³University of Arizona, Tucson, Arizona
- MOF am 10:10 **TargetSeeker-MS: A Bayesian Inference Approach for Drug Target Discovery using Protein Fractionation Coupled to Mass Spectrometry;** Mathieu Lavallée-Adam¹; Alexander Pelletier^{1,2}; Jolene K. Diedrich^{1,3}; William Low³; Michael Petrascheck¹; James J. Moresco^{1,3}; John R. Yates III^{1,3}; ¹The Scripps Research Institute, La Jolla, CA; ²UCSD, La Jolla, CA; ³The Salk Institute, La Jolla, CA

**8:30-10:30 am MONDAY
METABOLOMICS: UNTARGETED PROFILING**

Corey D. Broeckling (Colorado State University)

Hemisfair Ballroom 2, level 3

- MOG am 08:30 **Automated Solid Phase Extractions Coupled with Ion Mobility-Mass Spectrometry Analyses Allow Rapid Metabolomic Screening of Complex Plasma and Urine Samples;** Erin S. Baker¹; Xing Zhang²; Xueyun Zheng¹; Kristin E. Burnum-Johnson¹; Jennifer E Kyle¹; Young-Mo Kim¹; Erika M. Zink¹; Matthew E Monroe¹; Yehia M Ibrahim¹; Daniel J Orton¹; Justin G. Teeguarden¹; Thomas O Metz¹; Richard D. Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Colorado, Denver, CO
- MOG am 08:50 **Untargeted Profiling with Single-cell MS Uncovers Small-Molecule Cell Heterogeneity along the Left-Right Body Axis in the Frog Embryo;** Rosemary Masu Onjiko¹; Sydney E Morris¹; Sally A Moody²; Peter Nemes¹; ¹Department of Chemistry, The George Washington University, Washington, DC; ²Department of Anatomy & Regenerative Biology, The George Washington University, Washington DC, DC
- MOG am 09:10 **Metabolomics: Elemental Composition from Ultrahigh Resolution FT-ICR MS; Structure from Two-Dimensional 1H/13C NMR Spectroscopy;** Alan G. Marshall¹; Lidong He²; Lissa C Anderson³; Christopher L Hendrickson³; Cheng Wang⁴; Lei Bruschweiler Li⁴; Dawei Li⁴; Rafael Bruschweiler⁴; ¹Ion Cyclotron Resonance Prog, Tallahassee, FL; ²Florida State University, Tallahassee, Florida; ³National High Magnetic Field Laboratory, Tallahassee, FL; ⁴Ohio State University, Columbus, OH
- MOG am 09:30 **High-Throughput Discovery of New Natural Products and Their Biosynthetic Gene Clusters using a Metabologenomics Approach;** Anthony Goering¹; Ryan A McClure²; James R Doroghazi³; Kou-San Ju³; Jessica C. Albright²; Nicole Haverland²; Yongbo Zhang²; Regan J Thomson²; William W Metcalf³; Neil L Kelleher²; ¹Northwestern University,



MONDAY MORNING ORAL SESSIONS

- Chicago, IL; ²Northwestern University, Evanston, IL; ³University of Illinois at Urbana-Champaign, Urbana-Champaign, IL
- MOG am 09:50 **Untargeted Stable-isotope Tracing of Folate-mediated 1-C Trafficking in Cancer Cells and an *in vitro* 3Dmodel of Neural Tube Closure**; Qiuying Chen¹; Amanda K Vaughn²; John W Steel²; Robert M Cabrera²; Richard H Finnell²; Steven Gross¹; ¹Weill Medical College of Cornell, New York, NY; ²University of Texas at Austin, Austin, TX
- MOG am 10:10 **Integration of Personal Metabolome and other Omes: Application to the Onset of Type 2 Diabetes**; Kevin Contrepois¹; Michael Snyder²; ¹Stanford University, Stanford, California; ²Stanford University School of Medicine, Palo Alto CA

8:30-10:30 am MONDAY MEMBRANE PROTEIN MS

**Nina Morgner (Johann Wolfgang Goethe-University)
Hemisfair Ballroom 1, level 3**

- MOH am 08:30 **Ion Mobility-Mass Spectrometry Reveals the Stoichiometry and Structures of Lipid Bound Amyloidogenic Peptide Complexes within Nanodiscs**; Richard A Kerr¹; Jukyung Kang¹; Anna Schwendeman¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- MOH am 08:50 **Surface Induced Dissociation Provides Insight into Membrane Protein-Lipid Interactions**; Sophie Harvey^{1,2}; Yang Liu³; Wen Liu³; Vicki Wysocki¹; Arthur Laganowsky³; ¹The Ohio State University, Columbus, Ohio; ²University of Manchester, Manchester, United Kingdom; ³Texas A&M Health Science Center, Houston, Texas
- MOH am 09:10 **Identification and Characterization of Small Membrane Protein Complex Subunits Presenting Challenges for Routine Mass Spectrometric Analysis**; Julian Langer¹; Anja Resemann²; Martin Kohlstaedt¹; Detlev Suckau²; Schara Safarian¹; Hartmut Michel¹; ¹MPI for Biophysics, Frankfurt Am Main, Germany; ²Bruker Daltonik GmbH, Bremen, Germany

- MOH am 09:30 **XL-FASP: A New Integrated Cross-Linking Workflow to Study Extra Large Membrane Protein Complexes**; Martial Rey¹; Eric Durand²; Eric Cascales²; Rémi Fronzes¹; Julia Chamot-Rooke^{1,3}; ¹Institut Pasteur, Paris, France; ²Institut de Microbiologie de la Méditerranée, CNRS, Marseille, France; ³CNRS, Paris, France
- MOH am 09:50 **Top-down and Middle-down High-Resolution Mass Spectrometry of Lipidated Proteins**; Julian Whitelegge¹; Joseph Capri¹; Whitaker Cohn¹; Don Puppione¹; Pasqual Liaux²; Frederic Halgand³; ¹University of California, Los Angeles Los Angeles, CA; ²Ruhr University Bochum, Bochum, Germany; ³University Paris Sud, Orsay, France
- MOH am 10:10 **Monitoring the Dynamic N-linked Cell Surface Glycoproteome by Quantitative Proteomics**; Christian Eberl¹; Mathias Kalxdorf¹; Stephan Gade¹; Marcus Bantscheff¹; ¹Cellzome GmbH a GSK company, Heidelberg, Germany

10:30 AM – 2:30 PM, MONDAY MONDAY POSTER SESSION Poster/Exhibit Hall

Lunch Concessions are open 11:00 am - 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

11:30 am – 1:00 pm Undergraduate Students

Meet the Experts at tables reserved for you
in Poster/Exhibit Hall.



2:30-4:30 pm MONDAY
FOOD SAFETY AND CHEMISTRY: FOODOMICS,
ALLERGENS, BACTERIA, FOODS
Katherine L. Fiedler (U.S. FDA)
Hall 1, level 1

- MOA pm 02:30 **SWATH vs. MRM for Food Safety -Using Advanced MS to Verify the Gluten-free Status of Barley**; Michelle Lisa Colgrave¹; Keren Byrne¹; Gregory Tanner²; Crispin Howitt²; ¹CSIRO Agriculture, Brisbane, Australia; ²CSIRO Agriculture, Canberra, Australia
- MOA pm 02:50 **Analyses of Human Milk Oligosaccharides Discover Factors that Enhance and Diminish Infant Growth**; Jasmine C. C. Davis¹; Sarah Totten²; Lauren D. Wu¹; Sridevi Krishnan¹; Mark R. Charbonneau³; Michael J. Barratt³; Jeffrey I. Gordon³; Angela M. Zivkovic¹; Carlito B. Lebrilla¹; ¹University of California, Davis, Davis, CA; ²Stanford University School of Medicine, Palo Alto CA; ³Washington University in St. Louis, St. Louis, MO
- MOA pm 03:10 **Risk Verses Benefits for Cadmium, Lead and Mercury Exposure From Seafood Consumption**; Marc E. Engel; FDACS, Tallahassee, FL
- MOA pm 03:30 **Chemical Changes in a Gamma Ray-Irradiated Rodent Diet Revealed by nanoLC-MS/MS**; Jeevan K Prasain¹; Landon Wilson¹; Clinton J Grubbs¹; Stephen Barnes¹; ¹University of Alabama at Birmingham, Birmingham, AL
- MOA pm 03:50 **Investigation of Sample Preparation and Data Acquisition Effects on Non-Targeted Screening of Food Matrices Using LC/HR-MS**; Ann M Knolhoff¹; Caitlin Kneapler¹; Timothy R Croley¹; ¹FDA/CFSAN, College Park, MD
- MOA pm 04:10 **Forensic Analysis of a Mass Poisoning in Mozambique Associated with a Homebrewed Beverage using LC-HRAM MS and DART-MS**; Sara Kern¹; Travis M. Falconer¹; Jennifer L Brzezinski¹; Brian L Boyd¹; James A Turner¹; Jonathan J Litzaul¹; ¹US FDA, Cincinnati, OH

2:30-4:30 pm MONDAY
FUNDAMENTALS: ION SPECTROSCOPY
Thomas Rizzo (École Polytechnique Fédérale de Lausanne (EPFL))
Room 221, level 2

- MOB pm 02:30 **Structural Transitions in Gas Phase Proteins Investigated via IR Spectroscopy: from Native to Helical to Unzipped**; Isabel Gonzalez¹; Eike Mucha¹; Jongcheol Seo¹; Waldemar Hoffmann¹; Stephan Warnke¹; Kevin Pagel^{1,2}; Gert Von Helden¹; ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; ²Freie Universität Berlin, Berlin, Germany
- MOB pm 02:50 **Understanding Structures of Amino Acid Cluster Ions in the Gas Phase: Solved and Unsolved Problems**; Xianglei Kong; Nankai University, Tianjin
- MOB pm 03:10 **Conformation-specific IR-UV Double-resonance Spectroscopy and Structural Analysis of Sodiated Leucine Enkephalin**; Nicole Burke¹; Christopher Harrilal¹; Andrew DeBlase¹; Timothy Zwierni¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MOB pm 03:30 **Action-Excitation Energy Transfer for the Structural Characterization of Proteins**; Nathan Hendricks¹; Ryan R Julian²; ¹University of California, Riverside, Riverside, CA; ²University of California, Riverside Riverside, CA

- MOB pm 03:50 **Gas-phase VUV Photoionization and Photofragmentation of Geometrically Well-Defined Coinage Metal Nanocluster Cations**; Richard A. J. O'hair¹; Steven Daly²; Athanasios Zavras³; Laurent Nahon⁴; Jiaye Li⁵; Alexandre Giuliani⁴; Rodolphe Antoine²; Philippe Dugourd^{2,6}; ¹University of Melbourne, Victoria, Australasia; ²Université Lyon, Lyon, France; ³University of Melbourne, Melbourne, Australia; ⁴SOLEIL, l'Orme des Merisiers, St Aubin, Gif sur Yvette Cedex, France; ⁵University of Melbourne, Victoria, Australia; ⁶CRNS, Lyon, France
- MOB pm 04:10 **Near-UV Water Splitting by Gas-Phase Copper(bipy) Complexes**; Andy Dang¹; Frantisek Turecek¹; Christopher J Shaffer²; Victor Ryzhov³; Michael Lesslie³; John Lawler³; ¹University of Washington, Seattle, WA; ²Valpar, Minneapolis, MN; ³Northern Illinois University, DeKalb, IL

2:30-4:30 pm MONDAY
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
W. Alexander Donald (University of New South Wales)
Stars Ballroom 1, level 3

- MOC pm 02:30 **Measuring Masses of Single Bacterial Whole Cells with Laser Induced Acoustic Desorption Plasma Charge Detection Quadrupole Ion Trap Mass Spectrometer**; Shao-Yu Liang¹; Chou-Hsun Han¹; Dineshkumar Yograj Turkar¹; Avinash Adhikar¹; Patil¹; Szu-Wei Chou^{1,2}; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng Hualien, Taiwan; ²AcroMass Technologies, Inc. Taipei, Taiwan
- MOC pm 02:50 **Near Field Ablation High Lateral Resolution Sampling for Mass Spectrometry**; Fan Cao¹; Fabrizio Donnarumma¹; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA
- MOC pm 03:10 **Ultra-Soft Picosecond Laser Extraction of Biological Compounds from Water and Tissue for Mass Spectrometry**; Wesley Robertson¹; Yinfei Lu¹; Cornelius L Pieterse¹; Frederik Busse¹; R.J.Dwayne Miller¹; ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- MOC pm 03:30 **Automated High Throughput Identification of Microorganisms using Rapid Evaporative Ionisation Time of Flight Mass Spectrometry (REIMS-ToF-MS)**; Zsolt Bodai¹; Daniel Simon²; Schaffer Richard²; Frankie Bolt¹; Tamas Karancsi²; Julia Balog²; Tony Rickards¹; Adam Burke¹; Simon Cameron¹; Kate Hardiman¹; Monica Rebec¹; Zoltan Takats¹; ¹Imperial College, London, United Kingdom; ²Waters Research Center, Budapest, Hungary
- MOC pm 03:50 **A Robotic Trapping Column Exchanger for Increasing Clinical Assay Throughput by Capillary Liquid Chromatography-Mass Spectrometry**; Sandra E. Spencer¹; Huilin Shi²; Thomas N. Corso³; Michael J MacCoss²; ¹Univ. of North Carolina at Chapel Hill, Chapel Hill, NC; ²University of Washington, Seattle, WA; ³CorSolutions, LLC., Ithaca, NY
- MOC pm 04:10 **Open Probe Fast GC-MS – Combining Ambient Sampling, Ultra-Fast Separation and In-Vacuum Ionization for Real Time Forensic Analysis**; Uri Keshet¹; Aviv Amirav²; Alexander B Fialkov¹; Tal Aloni¹; ¹Tel Aviv University, Tel Aviv, Israel; ²Tel-Aviv University, Tel-Aviv, Israel

2:30-4:30 pm MONDAY
ANTIBODIES AND ANTIBODY DRUG CONJUGATES
Shawna Hengel (Seattle Genetics, Inc.)
Stars Ballroom 2-3, level 3

- MOD pm 02:30 **Leveraging Antibody Structure Analysis via Data Multiplexing in Top-Down Targeted Protein analysis;** Kristina Srzentic¹; Konstantin Nagornov²; Anton N Kozhinov²; Yuri O Tsybin²; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ²Spectroswiss Sàrl, Lausanne, Switzerland
- MOD pm 02:50 **Extending the Middle-Down HDX-MS Method for Residue-Level Structural Characterization of Antibody-Antigen Complexes;** Jingxi Pan¹; Suping Zhang²; Christoph H. Borchers^{1,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²MRM Proteomics, Inc., Victoria, BC, Canada; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MOD pm 03:10 **A Modular and Adaptive Mass Spectrometry-Based Platform for Support of Bioprocess Development toward Optimal Host Cell Protein clearance;** Feng Yang¹; Donald E. Walker¹; Joseph Carver¹; David A. Michels¹; Christopher Yu¹; ¹Genentech Inc, South San Francisco, CA
- MOD pm 03:30 **Where Did the Linker-Payload Go? A Quantitative Investigation on the Destination of Released Linker-Payload from Antibody-Drug-Conjugate with Maleimide-Linker in Plasma;** Cong Wei¹; Guodong Zhang²; Tracey Clark¹; Frank Barletta¹; Nathan Tumey¹; Brian Rago¹; Steven Hansel¹; Xiaogang Han¹; ¹Pfizer, Groton, CT; ²Shire, Lexington, MA
- MOD pm 03:50 **Profiling Multiple Post-translational Modifications of Therapeutic Antibodies Circulating in Human Patients;** Yinyin Li¹; Michael Monine¹; Yu Huang¹; Patrick Swann¹; Yelena Lyubarskaya¹; ¹Biogen Inc., Cambridge, MA
- MOD pm 04:10 **Model-Based Algorithms for Intact Mass Analysis of Biotherapeutics;** Marshall W. Bern¹; Yong J Kil²; Eric Carlson¹; Doron Kletter¹; Wilfred Tang¹; Christopher Becker¹; ¹Protein Metrics, Palo Alto, CA; ²Protein Metrics, San Carlos, CA

2:30-4:30 pm MONDAY
DATA INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS
Andrew K. Ottens (Virginia Commonwealth University)
Stars Ballroom 3-4, level 3

- MOE pm 02:30 **LC-SWATH-MS/MS Data Acquisition with Deconvolution of High-Resolution MS Data in Metabolomics;** Tomas Cajka¹; Oliver Fiehn¹; ¹UC Davis Genome Center, Davis, CA
- MOE pm 02:50 **A Promising Alternative to SWATH:MS1-based Strategy(IonStar) Enables In-Depth and Reproducible Proteomics Quantification in Large Cohorts with High Accuracy and Extremely-Low-Level-Missing-Data;** Xiaomeng Shen^{1,2}; Jun Li³; Shichen Shen^{1,2}; Qiang Hu⁴; Xin Miao³; Chengjian Tu^{3,2}; Lei Nie⁵; Xue WANG⁴; Jianmin Wang⁴; William J Jusko³; Benjamin C Orsburn⁶; Jun Qu^{2,3}; ¹Dept. of Biochemistry at SUNY at Buffalo, Buffalo, NY; ²Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY; ³Dept. of Pharmaceutical Sci. at SUNY at Buffalo, Buffalo, NY; ⁴Roswell Park Cancer Institute, Buffalo, NY; ⁵Shandong University, Jinan, Shandong; ⁶Thermo Fisher Scientific, San Jose, CA

- MOE pm 03:10 **Qualitative and Quantitative Characterization of a Novel DIA Method for Omics Analysis and its Application to Biomedical Analyses;** Arthur Moseley¹; Chris Hughes²; Erik J. Soderblom³; Keith Richardson²; Will Thompson⁴; Jason Wildgoose²; James Langridge²; ¹Duke University School of Medicine, Durham, NC; ²Waters, Wilmslow, United Kingdom; ³Duke University School of Medicine, Durham, NC; ⁴Duke University School of Medicine, Durham, NC
- MOE pm 03:30 **Bidimensional FT-ICR MS: a fully Data Independent Acquisition;** Fabrice Bray¹; Lionel Chiron²; Matthias Witt³; Marc-André Delsuc⁴; Christian Rolando⁵; ¹Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France; ²CASC4DE, Strasbourg, France; ³Bruker Daltonic GmbH, Bremen, Germany; ⁴Université de Strasbourg, Strasbourg, France; ⁵Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq
- MOE pm 03:50 **Data Independent Acquisition for the Rapid Screening of de novo Protein Designs;** Jason Michael Gilmore¹; Jorge Fallas¹; George Ueda¹; David Baker¹; Michael J MacCoss¹; ¹University of Washington, Seattle, WA
- MOE pm 04:10 **High Content Discovery Proteomics of a Breast Tumor Tissue Microarray using Data Independent Acquisition;** Bin Fang¹; Douglas C Marchion¹; Amol Prakash²; Scott M Peterman³; Michelle Fournier¹; Zena Sayegh¹; Joseph J Johnson¹; Agnieszka Kasprzak¹; Daryoush Saeed-Vafa¹; Roohi Ismail-Khan¹; Steven A Eschrich¹; Anthony M Magliocco¹; John Koomen⁴; ¹Moffitt Cancer Center, Tampa, FL; ²Optys Tech Corporation, Philadelphia, PA; ³Thermo Fisher, San Jose, CA; ⁴H. Lee Moffitt Cancer Center, Tampa, FL

2:30-4:30 pm MONDAY
INFORMATICS: METABOLOMICS
Hyung Won Choi (National University of Singapore)
Hemisfair Ballroom 3, level 3

- MOF pm 02:30 **Collaborative Human Computing: The Next Generation Paradigm in Metabolomics;** Mingxun Wang^{1,2}; Pieter Dorrestein³; Nuno Bandeira^{1,2,3}; ¹Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; ²Computer Science and Engineering, University of California San Diego, La Jolla, CA; ³Skaggs School of Pharmacy, UC San Diego La Jolla, CA
- MOF pm 02:50 **FDR-controlled Metabolite Annotation for High-Resolution Imaging Mass Spectrometry;** Andrew Palmer¹; Michael Becker²; Ilya Chernyavsky³; Dominik Fay¹; Artem Tarasov¹; Vitaly Kovalev¹; Jens Fuchser²; Sergey Nikolenko¹; Theodore Alexandrov^{4,5}; ¹European Molecular Biology Laboratory, Heidelberg, Germany; ²Bruker Daltonic GmbH, Bremen, Germany; ³University of Bremen, Bremen, Germany; ⁴Skaggs School of Pharmacy, UC San Diego La Jolla, CA; ⁵SciLS GmbH, Bremen, Germany
- MOF pm 03:10 **Tandem Mass Spectral Libraries of Recurrent Unidentified Spectra for Urine and Plasma: A New Kind of Library for Metabolomics Applications;** Yamil Simon¹; Ramesh Marupaka²; Xinjian Yan²; Yuri Mirokhin²; Kelly H. Telu²; William E Wallace²; Stephen E Stein²; ¹NIST, Gaithersburg, MD; ²NIST, Gaithersburg MD
- MOF pm 03:30 **Hydrogen Rearrangement Rules for Computational MS/MS Fragmentation;** Hiroshi Tsugawa¹; Wataru Tanaka²; Ryo Nakabayashi¹;



Kazuki Saito^{1,3}; Masanori Arita^{1,4}; ¹RIKEN Center for Sustainable Resource Science, Yokohama, Japan; ²SOKENDAI, Mishima, Japan; ³Chiba University, Inage-ku, Japan; ⁴National Institute of Genetics, Mishima, Japan

MOF pm 03:50 **New in BioCyc: Pathway Collages and Pathway Prediction Algorithm**; Peter Karp; *SRI International, Menlo Park, CA*

MOF pm 04:10 **Normalization and Integration of Large-Scale Mass Spectrometry-based Metabolomics Data Using Support Vector Regression**; Xiaotao Shen¹; Zhengjiang Zhu¹; *1*IRCB, Chinese Academy of Sciences, Shanghai, China

**2:30-4:30 pm MONDAY
NUCLEIC ACID MS**

**Silvia Balbo (University of Minnesota)
Hemisfair Ballroom 2, level 3**

MOG pm 02:30 **RNA Modification Mapping from Multiple Bacteria in a Single Sample using LC-MS/MS**; Xiaoyu Cao¹; Patrick A Limbach²; *1*University of Cincinnati, Cincinnati, Ohio; *2*University of Cincinnati, Cincinnati, OH

MOG pm 02:50 **Exploring the Use of Top-Down Mass Spectrometry for the Identification, Localization, and Relative Quantitation of RNA Nucleobase Methylations**; Heidelinde Glasner¹; Christian Riml²; Christoph Falschlunger²; Ronald Micura²; Kathrin Breuer²; ¹Innsbruck, Tyrol; ²University of Innsbruck, Innsbruck, Austria

MOG pm 03:10 **Cation Binding to Nucleic Acids**; Adrien Marchand¹; Clémence Rabin¹; Sandrine Livet¹; Solenne Delahaye¹; Valentina D'Atri¹; Josephine Abi-Ghanem¹; Frédéric Rosu²; Valerie Gabelica¹; *1*Univ. Bordeaux / Inserm / CNRS (ARNA Laboratory), IECB Pessac, France; *2*CNRS UMS 3033, IECB Pessac, France

MOG pm 03:30 **Plasticity in Cancer Nucleotide Metabolism Revealed by Multiplexed MRM Assays**; Thuc Le¹; Soumya Poddar¹; Joseph Capri¹; Evan Abt¹; Woosuk Kim¹; Julian P Whitelegge¹; Kym F Faull¹; Caius Radu¹; *1*UCLA, Los Angeles, CA

MOG pm 03:50 **Identification and Characterizations of 8,5'-cyclo-2'-deoxypurine Lesion-binding Proteins**; Preston Williams¹; Pengcheng Wang¹; Yinsheng Wang¹; *1*University of California - Riverside, Riverside, CA

MOG pm 04:10 **Multi-Class Carcinogenic DNA Adduct Quantification in Formalin-Fixed Paraffin-Embedded Tissues by Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry**; Jingshu Guo¹; Byeong Hwa Yun¹; Pramod Upadhyaya¹; Lihua Yao¹; Sessa Krishnamachari¹; Thomas A. Rosenquist²; Arthur P. Grollman²; Robert J. Turesky¹; *1*University of Minnesota, Minneapolis, MN; *2*Stony Brook University, Stony Brook, NY

2:30-4:30 pm MONDAY

**COVALENT LABELING AND CHEMICAL CROSSLINKING
Juri Rappsilber (University of Edinburgh and TU Berlin)
Hemisfair Ballroom 1, level 3**

MOH pm 02:30 **Crosslink-assisted Structure Determination of the Human Spliceosomal Subcomplex, U4/U6.U5 tri-snRNP**; Olexandr Dybkov¹; Romina V. Hofe^{1,2}; Dmitry E. Agafonov¹; Berthold Kastner¹; Wen-Ti Liu¹; Holger Stark^{1,3}; Reinhard Luehrmann¹; Henning Urlaub^{1,2}; *1*Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; *2*University Medical Center (UMG), Goettingen, Germany; *3*Georg-August-Universitaet Goettingen, Goettingen,

Germany

MOH pm 02:50 **Developing a New Quantitative Cross-linking Mass Spectrometry (XL-MS) Strategy to Define *in vivo* Structural Dynamics of Protein Complexes**; Clinton Yu¹; Xiaorong Wang¹; Rosa I Viner²; Alex Huszaghi¹; Eric Novitsky¹; Tonya Second²; Scott Rychnovsky¹; Lan Huang¹; *1*University of California, Irvine, Irvine, CA; *2*Thermo Fisher Scientific, San Jose, CA

MOH pm 03:10 **Solving the Tertiary Structure of SalBII Protein by Chemical Cross-Linking/Mass Spectrometry and Molecular Modeling**; Allan Jhonathan Ramos Ferrari¹; Hugo Cesar de Jesus¹; Marcio Vinicius Bertacine Dias²; Luciana Gonzaga de Oliveira¹; Peter Leadlay³; Fabio Cesar Gozzo¹; *1*University of Campinas, Campinas, Brazil; *2*University of São Paulo, São Paulo, SP; *3*University of Cambridge, Cambridge, UK

MOH pm 03:30 **Combining Zero-Length Cross-Linking and Label-free Proteomics to Identify Functional Binding Residues in an Ordered-Disordered Heterodimeric Protein Complex**; Michelle Dubuke¹; Stephanie Maniatis¹; Mary Munson¹; Scott A Shaffer¹; *1*UMass Medical School Department of Biochemistry and Molecular Pharmacology, Worcester, MA

MOH pm 03:50 **Charting the Cellular Interactome by Proteome-Wide Cross-Linking Mass Spectrometry**; Fan Liu¹; Philip Lossi¹; Richard Scheltema¹; Rosa Viner²; Albert Heck¹; *1*Utrecht University, Utrecht, The Netherlands; *2*Thermo Fisher Scientific, San Jose, CA

MOH pm 04:10 **Global XL-MS: Proteome-scale Interactomes Unifying Cross-Linked Datasets**; Devin Schweppe¹; Chunxiang Zheng¹; Juan Chavez¹; Arti Navare¹; Xia Wu¹; Jimmy K Eng¹; James Bruce¹; *1*University of Washington, Seattle, WA

**4:45 - 5:30 PM, MONDAY AFTERNOON
AWARD LECTURE
Jenny Brodbelt (University of Texas, Austin) presiding
Hall 1, level 1**



Award for a Distinguished Contribution in Mass Spectrometry

Scott A. McLuckey
Purdue University

There are light refreshments in common areas.

01 Top-Down Proteomics: Ready for Primetime?

Ying Ge and Paul Thomas presiding
Room 220, level 2

Top Down protein mass spectrometry allows comprehensive analysis of intact, multiply modified proteoforms from complex mixtures. In this workshop, we will provide an update from the Consortium for Top Down Proteomics, discussing new community-wide pilot projects. We will also review and discuss common roadblocks to successful top down proteomics experiments from sample preparation to data acquisition to data analysis in a panel format. A limited number of 5 minute 'lightning talks' will be available for researchers to provide rapid-fire updates on recent achievements and accomplishments of note. Contact workshop chairs if you are interested in presenting.

02 Next Generation LC-MS: Critical Insights & Future Perspectives

Hongying Gao presiding
Room 221, level 2

Recent advancement in high resolution mass spectrometry has expanded the capabilities of the instrumentation for both qualitative and quantitative analysis. Coupling UPLC with HRMS, samples can be analyzed without authentic standards nor the knowledge of the analytes in the samples, and data can be banked for post-acquisition data processing when the knowledge of the analytes or the authentic standards becomes available. The ideal super LC/MS technology needs to capture the quantitative and qualitative information of the unknown analytes with a variety of physiological properties in a wide range of chemical space. This data banking approach presents new challenges and opportunities for high resolution LC/MS system. In this workshop, a case in industry will be presented to illustrate the need for advancement in LC and mass spectrometry, and then the latest technology advances in high resolution LC/MS and ion mobility will be presented, followed by open discussions on the capabilities and feasibility of the features of next generation LC/MS. Introduction and Objectives of the Session. Why We Need Super LC/MS System? Hongying Gao, Pfizer Inc. Challenges and Opportunities in High Resolution LC/MS. Alexander Makarov, Thermo Fisher Scientific. How the Rise of IMS Will Change the Use of LC/MS. Richard (Dick) D. Smith, Pacific Northwest National Laboratory.

03 Art and Cultural Heritage Mass Spec Applications

Mehdi Moini presiding
Room 225A, level 2

The purpose of this workshop is to discuss the application of 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 museums' specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of paint, coating and binders; textiles; bone and tissue; ink and paper. 2) Mechanism of aging and degradation of art and natural history objects. 3) Dating. 4) Impact of radiation on museums' specimens. 5) Fossilomics and ancient DNA. 6) Forensic archeology. 7) Species identification of proteinaceous materials used in work of art and natural history. 8) Identification of forgery.

04 Bioinformatics: Challenges & Opportunities in Proteogenomics (Bioinformatics for MS)

Sangtae Kim and Meena Choi presiding
Room 225B, level 2

Proteogenomics (integrated proteomics and genomics) has gained lots of popularity in recent years. Traditionally, it was mainly used to improve genome annotation of newly or partially sequenced organisms, but now it is also increasingly applied in cancer studies. In this workshop, we will discuss bioinformatics challenges and opportunities in proteogenomics. It will begin with short introductory presentations by researchers who have recently conducted large-scale proteogenomics studies, and be followed by audience driven discussions.

05 Environmental Analysis: Emerging Topics (Environmental Applications Interest Group)

Achille Cappiello, Marc E. Engel, and
Christopher G. Gill presiding
Room 225C, level 2

This workshop will feature three or four members of the environmental mass spectrometry community that will informally present a maximum of five slides to generate discussion within the working group. Topic areas for the workshop this year are centered upon emerging contaminants (targeted and non targeted) as well as new analytical approaches for their characterization and measurement.

06 Metal Cationization in MS/MS of Biomolecules (Metal Ion Coordination Chemistry Interest Group)

Alexandre Shvartsburg and Cheng Lin presiding
Room 225D, level 2

A viable alternative to the prevailing paradigm of ionizing biomolecules by protonation (or deprotonation) is the addition of other charged moieties. Metal cationization commonly introduces distinct isotopic patterns, major conformational changes, novel electronic properties, and/or new dissociation chemistry (especially in electron activated mechanisms) that present diverse and still sparsely explored analytical opportunities. In tandem mass spectrometry, metalation has been employed to stabilize labile modifications, promote complementary and more informative fragmentation pathways, and facilitate isomer separation. In another aspect, the native structure of many biomolecules that is often desirable to preserve in MS depends on the metal coordination. This workshop will encourage the adoption of metal cationization in biological mass spectrometry and particularly MS/MS applications.

07 Proteomics Informatics for the Trans-Proteomic Pipeline

Luis Mendoza and Eric Deutsch presiding
Room 301A, level 3

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on 5 individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topic leads for discussion are: cross-linking analysis with Kojak, label-free quantitative analysis with StPeter, chimeric spectrum analysis with reSpect, proteomics informatics using cloud computing infrastructure such as Amazon Web Services, and analysis of SWATH-MS data with SWATHProphet. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

08 Metabolomics: Emerging Technologies for Continued Innovation (Metabolomics Interest Group)

Timothy Garrett and Andrew Patterson presiding
Room 301BC, level 3

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) advances in chromatographic separation of metabolites and its influence on metabolomics data, (ii) innovative experimental designs, and (iii) new tools for metabolite identification.

**09 Polymer MS Technology: Advancements and Discussion
(Polymeric Materials Interest Group)
Stephen Rumbelow and Gyorgy Vas presiding
Room 302A, level 3**

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 for both characterization and quantitation of oligomeric species. 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, and different type of products such as packaging and medical devices.

**10 MS Analysis of Antibody-Drug Conjugates
(Pharmaceuticals Interest Group)
Christine Gu and Matthew Schenauer presiding
Room 302BC, level 3**

Due to the success of pharmaceutical interest group workshops since 2013, and continued interest in MS analysis of antibody drug-conjugates (ADCs), we propose a similar workshop for 2016. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis in the industry for the discovery and development. Potential areas of discussion may include the large range of characterization required for ADCs from initial MAB assessment to bioanalytical assay development, with the focus on Mass Spec method development and optimization. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

**11 Protocol Repositories for Proteomics and Metabolomics
(Analytical Lab Managers Interest Group)
Allis Chien and Brett Phinney presiding
Room 303A, level 3**

Protocols and SOP's are the lifeblood of any analytical core facility. Although finding detailed protocols has gotten easier over the years (Nature Protocols for example), finding protocols that have been validated, via successful use by numerous people, is still challenging and fraught with failure. Often even following a detailed published protocol can fail and the user is left wondering: What happened? In this workshop we will discuss options for finding and using protocol repositories for mass spectrometry-based analytical core facilities (Proteomics and Metabolomics). Specifically, we will discuss the new protocol repository set up by the Association of Biomolecular Resource Facilities (ABRF) along with several other freely available options.

**12 Miniaturization of Ion Traps and Related Devices
(Ion Trap Interest Group)
Daniel Austin and Zheng Ouyang presiding
Room 303BC, level 3**

Ion traps constitute a major portion of the effort to produce miniaturized mass spectrometers. In addition, the wealth of new ionization techniques have led to many new devices for introduction, transmission, and detection of ions in the context of portable devices. The workshop will start with short (4-minute) snippets from several groups working in this area. Next, a panel-led discussion will address opportunities, applications, and challenges of portable mass spectrometry.

**13 MS Career Options: How to Kick-Start your Career
(Young Mass Spectroscopists Interest Group)
Kristin Wildsmith and Violet Lee presiding
Room 304, level 3**

The workshop features an interactive panel discussion on professional development (Bring your questions). Topics will be centered around career planning and management, fundamental training, industrial

internship, and diversity of career options within the MS field. A panel of representatives from government, industrial (domestic and foreign) and academic organizations, will share their knowledge, experience, and practices on career prospects.

**14 System Performance: Tracking through Statistical QC
Monitoring (LC/MS & Related Topics Interest Group)
Michael Bereman and Brent Dixon presiding
Room 305, level 3**

Liquid chromatography mass spectrometry systems are recognized as highly sensitive and specific tools for metabolomic and proteomic analyses. Ensuring the integrity of data through a system of controls referred to as quality control standards enables a higher level of confidence in the obtained results. Providing intra-laboratory personnel with quality control charts allows for correction when standards exceed acceptability limits. Control charts may be used in an inter-laboratory manner to compare results across labs. By monitoring performance standards, a higher level of commutability of experimental results may be achieved.

The workshop will provide a demonstration of online QC tracking through Skyline; system performance tracking and control charting. The workshop will explore available controls for tryptic digestion to ensure proteolytic cleavage. The content will also include a section related to metabolomic analyses.

Integrating quality control and performance standards in the experimental design is not a new concept. However, the intention to monitor these standards over time and across experiments presents an opportunity. A major limitation in the broader analysis of experimental control performance has been aggregation and visualization. Precious samples may be better utilized by identifying a trend and performing a preventive action to avoid a failed assay. The overall aim is to shift to a prospective action driven review rather than a retrospective control review approach.

**AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL**

8:30-10:30 am TUESDAY
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION
AND METHOD DEVELOPMENT
Young Jin Lee (Iowa State University)
Hall 1, level 1

- TOA am 08:30 **Petroleomic Characterization using an Ion Mobility-Orbitrap Platform;** Yehia Ibrahim¹; Roza Wojcik²; Spencer A Prost²; Sandilya Garimella²; Randolph Norheim²; Erin Baker²; Noor Aly²; Hans Ketelslegers³; Fabian Grimm⁴; Ivan Rusyn⁴; Richard D Smith²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA; ³Concawe, Brussels, BELGIUM; ⁴Texas A&M, College Station, TX
- TOA am 08:50 **Molecular Composition of Petroleum Interfacially Active Species: Implications in Emulsion Science;** Ryan P. Rodgers¹; Amy C Clingenpeel^{2,3}; Winston K Robbins⁴; Steven Rowland⁴; Yuri E Corilo^{3,4}; David C Podgorski⁴; ¹Nat'l High Magnetic Field Lab, Tallahassee, FL; ²FSU Department of Chemistry and Biochemistry, Tallahassee, FL; ³National High Magnetic Field Laboratory, Tallahassee, FL; ⁴Future Fuels Institute, FSU Tallahassee, FL
- TOA am 09:10 **Gas-phase Hydride Transfer between Carbocations and Analyte Alkanes Provides a Gentle and Controllable Ionization Method with Minimal Fragmentation;** Mingzhe Li¹; Chunfen Jin¹; Hanyu Zhu¹; Mark Romanczyk¹; Jyrki Viidanoja²; Hilikka I Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Neste Oil, Keilaranta, Finland
- TOA am 09:30 **Selective Analysis of Complex Crude Oil Mixtures using Chemical and Instrumental Methods;** Wolfgang Schrader¹; Alessandro Vetere¹; Xuxiao Wang¹; ¹Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany
- TOA am 09:50 **Gel Permeation Chromatography (GPC) Inductively Coupled Plasma High Resolution Mass Spectrometry (ICP HR MS) Parameters Study in Petroleum Product Analysis;** Sara Gutierrez Sama^{1,2}; Alain Desprez^{1,2,3}; Gabriel Krier³; Charles-Philippe Lienemann⁴; Jérémie Barbier⁴; Ryszard Lobinski¹; Caroline Barrere-Mangote^{2,5}; Pierre Giusti^{2,5}; Brice Bouyssiere^{1,5}; ¹CNRS/UPPA, UMR 5254, LCABIE, Pau, France; ²TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; ³UL, LCP-A2MC, Metz, France; ⁴IFPE, Solaize, France; ⁵TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, -, France
- TOA am 10:10 **Online Photoionization Time-of-Flight Mass Spectrometric Study on the Catalytic Pyrolysis of Bituminous Coal over HUSY and HZSM-5;** Yanan Zhu¹; Jiuzhong Yang¹; Fei Qi²; Yang Pan¹; ¹University of Science and Technology of China/USTC, Hefei, P.R. China; ²Shanghai Jiao Tong University, Shanghai, China

8:30-10:30 am TUESDAY
FUNDAMENTALS: METAL ION CATIONIZATION,
METAL-LIGAND INTERACTIONS AND CATALYSIS
Jinhua Ren (University of the Pacific)
Room 221, level 2

- TOB am 08:30 **Chemi-ionization Thermochemistry of the Lanthanides: Relevance for Atmospheric Release Studies;** Peter B. Armentrout¹; Maria Demireva¹; Cameron Owen¹; Richard M Cox²; ¹University of Utah, Salt Lake City, UT; ²Pacific Northwest National Lab, Richland, WA

- TOB am 08:50 **Supermetallization of Peptides and Proteins;** Yury Kostyukevich¹; Alexey S Kononikhin²; ³Maria Indeykina^{4,3}; Evgeny Kukaev^{2,4}; Igor A Popov^{4,5}; Eugene Nikolaev^{1,2,3,4}; ¹Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; ²Moscow Institute of Physics and Technology, Moscow, Russia; ³Institute for Energy Problems of Chemical Physics, Moscow, Russia; ⁴Emanuel Institute of Biochemical Physics, Moscow, Russia; ⁵Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia
- TOB am 09:10 **Copper-binding and Redox Activity and of a Series of Alternative Methanobactin Peptides;** Laurence Angel¹; Yashodharani Vytla¹; Manogna Deeconda¹; Sravya Challa¹; Rajpal Vangala¹; Jacob W McCabe¹; ¹Department of Chemistry, Texas A&M University-Commerce, Commerce, TX
- TOB am 09:30 **Capture of Reactive Monophosphine Ligated Palladium(0) Intermediates by Mass Spectrometry;** Qiuling Zheng¹; Yong Liu²; Qinghao Chen²; Meihong Hu¹; Roy Helmy²; Edward Sherer²; Christopher Welch²; Hao Chen¹; ¹Ohio University, Athens, OH; ²Merck, Darmstadt, Germany
- TOB am 09:50 **Revisiting Organometallic Chemistry by Ion Mobility;** Izabella Czerwinska¹; Sophie Rappe¹; Carlos Larriba-Andaluz²; Nicolas Smargiasso¹; Christopher Kune¹; Albert Demonceau³; Johann Far¹; Lionel Delaude³; Edwin A De Pauw¹; ¹Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; ²Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; ³Laboratory of Catalysis, University of Liege, Belgium
- TOB am 10:10 **Testing Nanoscale Homogeneity with Massive Cluster Secondary Ion Mass Spectrometry;** Michael J Eller¹; Stanislav V Verkhoturov¹; Emile A Schweikert¹; ¹Texas A&M University, College Station, TX

8:30-10:30 am TUESDAY
HRMS FOR QUANTITATION IN DRUG DISCOVERY,
DEVELOPMENT AND BEYOND
Ashley Ruth (FDA/DPA)
Stars Ballroom 1, level 3

- TOC am 08:30 **Analysis of Host Cell Proteins throughout Biopharmaceutical Purification;** Martha Stapels¹; Michelle Busch¹; Samantha Cooper¹; Veena Warikoo¹; Kate Zhang¹; ¹Sanofi Genzyme, Framingham, MA
- TOC am 08:50 **Exploring the Use of HRMS for Circumventing Complex and Lengthy Sample Pre-Treatment for Absolute Quantification of mAbs in Plasma/Serum Samples;** Ulrik Hvid Møstard^{1,2}; Tam T. T. Nguyen¹; Amaury Herbet²; Narciso Costa²; Didier Boquet²; Christophe Junot²; François Becher²; Kasper Dyrberg Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²CEA Saclay, DSV/iBiTec-S/LEMM, Gif sur Yvette, France
- TOC am 09:10 **Evaluation of Ion Mobility and Targeted QToF Acquisition Modes for the Quantitative Analysis of Peptides;** Jayne Kirk¹; Mark Wrona²; Kelly Doering²; Russell Mortishire-Smith¹; Lisa A Vasicek³; Kevin P Bateman³; ¹Waters Corporation, Wilmslow, UK; ²Waters Corporation, Milford, MA; ³Merck & Co., West Point, PA
- TOC am 09:30 **Bioanalysis and in vivo Stability Evaluation of a PEGylated Protein Drug by UHPLC-HRMS using a Disulfide-Containing Surrogate Peptide;** Naiyu Zheng¹; Jianing Zeng¹; Amy Manney¹;



Lakenya Williams¹; Anne-Françoise Aubry¹; Kimberly Voronin¹; Adela Buzescu¹; Yan J Zhang¹; Alban Allentoff¹; Carrie Xu¹; Hongwu Shen¹; William Warner¹; Mark E Arnold¹; ¹Research and Development, Bristol-Myers Squibb Company, Princeton, NJ

TOC am 09:50 **High-throughput MALDI TOF Mass Spectrometry for Drug Discovery in the Ubiquitin Pathway;** Virginia De Cesare¹; Axel Knebel¹; Matthias Trost¹; ¹MRC PPU, University of Dundee, Dundee, United Kingdom

TOC am 10:10 **Simultaneous Quantitation and Metabolite Profiling of RG-125, a GalNAc-conjugated Oligonucleotide, and Its Five Metabolites using HRAM LC/MS;** Brandon Wilcock¹; Kai Liu²; Daniel J. Mauchley¹; Min Meng¹; Troy Voelker¹; Brian P. Schultz²; Tate Owen²; John Grundy²; ¹Covance, Salt Lake City, UT; ²Regulus Therapeutics Inc., San Diego, CA

8:30-10:30 am TUESDAY
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Wendell P. Griffith (University of Texas at San Antonio)
Stars Ballroom 2-3, level 3

TOD am 08:30 **Design and Optimization of a Fully-controlled Stainless Steel Sublimator for Matrix Deposition in MALDI-IMS Experiments;** Roberto Fernández¹; Jone Garate¹; Sergio Lage¹; Jose A Fernandez¹; ¹University of Basque Country, UPV/EHU Leioa Basque Country, Spain

TOD am 08:50 **Identification of Bio-Molecules at Sub-Micron Lateral Resolution by TOF-SIMS Parallel Imaging MS/MS;** Gregory L. Fisher¹; Nina Ogrinc Potocnik²; Anne L Bruinen²; John S Hammond¹; Ron M.A. Heeren²; ¹Physical Electronics, Chanhassen, MN; ²Maastricht University, M4I, Maastricht, Netherlands

TOD am 09:10 **Developing a Gas Cluster Ion Beam (GCIB) for Enhanced Ionization and Reduced Matrix Effects in Secondary Ion Mass Spectrometry (SIMS);** Hua Tian¹; Andreas Wucher²; Nicholas Winograd¹; ¹Pennsylvania State University, University Park, PA; ²University of Duisburg-Essen, Essen, Germany

TOD am 09:30 **Ultra-High Spatial Resolution AP-SMALDI Mass Spectrometry Imaging of Lipids;** Mario Kompauer¹; Sven Heiles¹; Bernhard Spengler¹; ¹Justus Liebig University, Giessen, Germany

TOD am 09:50 **Forensic Analysis of Latent Fingermarks by Silver-Assisted LDI Imaging MS on Non-Conductive Surfaces;** Nidia Lauzon¹; Martin Dufresne²; Alexandre Beaudoin³; Pierre Chaurand²; ¹University of Montreal, Montreal, Canada; ²University of Montreal, Montreal Qc, Canada; ³Sûreté du Québec, Montreal Qc, Canada

TOD am 10:10 **Quantitative Imaging of Gold Nanoparticles in Tissues using inkjet-Printed Standards;** Sukru Gokhan Elci¹; Brian Creran¹; Bradley Duncan¹; Alyssa L M Marsico¹; Vincent M Rotello¹; Richard W Vachet¹; ¹University of Massachusetts, Amherst, MA

8:30-10:30 am TUESDAY
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY
Stephanie Cologna (University of Illinois, Chicago)
Stars Ballroom 4, level 3

TOE am 08:30 **Diacylglycerol Metabolism in Regulation of Innate and Adaptive Functions of Dendritic Cells;** Ku-Lung Hsu¹; Myungsun Shin¹; ¹University of Virginia, Charlottesville, VA

TOE am 08:50 **A Systems Approach to Define the Spatial-Temporal Dynamics of Host Organelles upon**

Viral Infection; Pierre Jean Beltran¹; Rommel Mathias¹; Ileana M. Cristea¹; ¹Princeton University, Princeton, NJ

TOE am 09:10 **Analysis of Proteomic Variation in the Human Population: The HipSci iPS Cell Project;** Dalila Bensaddek¹; Alejandro Brenes Murillo¹; Helena Kilpinen²; Angela Goncalves³; Mariya Chhatiwala⁴; Rachel Nelson⁵; Chris Kirton⁵; Ludovic Vallier⁴; Daniel Gaffney³; Oliver Stegle²; Richard Durbin³; Angus Iain Lamond¹; ¹University of Dundee, Dundee, UK; ²European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus, Cambridge, UK; ³Wellcome Trust Sanger Institute, Wellcome Trust Genome Campus, Cambridge, UK; ⁴Pancreatic Genetics, Wellcome Trust Genome Campus, Cambridge, UK; ⁵Cellular Generation & Phenotyping, CGaP, Wellcome Trust Sanger Institute, Cambridge, UK

TOE am 09:30 **Interrogating Oncogenic B-Raf Signaling through microRNAs using Functional Proteomics;** Thomas Lee^{1,2}; Nan Wang^{1,2}; Stephane Houel^{1,3}; Kasey L. Coutts¹; Natalie G. Ahn¹; ¹University of Colorado, Boulder, Colorado; ²University of Alberta, Edmonton, Canada; ³Thermo Fisher Scientific, San Jose, CA

TOE am 09:50 **Correlation of KRAS Proteoform Expression Profiles to Cancer Phenotypes via Integrated Proteogenomic Analysis of Colorectal Tumors;** Ioanna Ntai¹; Josiah E Hutton²; Richard D Leduc¹; Ryan T Fellers¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Vanderbilt University, Nashville, TN

TOE am 10:10 **Hunting Biomass Degrading Enzymes and Their Active Proteoforms through an Activity-Correlated Quantitative Proteomics Platform;** Hongyan Ma¹; Delafield Graham Daniel¹; Zhe Wang¹; Si Wu¹; ¹University of Oklahoma, Norman, OK

8:30-10:30 am TUESDAY
INSTRUMENTATION: NON-FT BASED ANALYZERS
Michael Westphall (University of Wisconsin-Madison)
Hemisfair Ballroom 3, level 3

TOF am 08:30 **Application of Multi Frequency Waveforms for Ion Isolation and Enhancement with the MOMA Ion Trap Mass Spectrometer;** Ryan M Danell¹; Andrej Grubisic²; Friso H W Van Amerom³; Veronica T Pinnick⁴; Xiang Li⁴; Stephanie Getty⁵; Ricardo Arevalo⁶; William Brinkerhoff⁶; ¹Danell Consulting, Inc., Winterville, NC; ²Center for Research and Exploration in Space Science and Technology (CRESTT), University of Maryland, College Park, MD; ³Mini-Mass Consulting, Inc., Hyattsville, MD; ⁴Center for Research and Exploration in Space Science and Technology (CRESTT), University of Maryland, Baltimore County, MD; ⁵NASA Goddard Space Flight Center, Greenbelt, MD

TOF am 08:50 **Second Order Space and Velocity Focusing Time of Flight Mass Spectrometry using an Accelerator Field Free Region;** Robert E. Haufler¹; Bill Loyd²; ¹AB Sciex, Concord, ON; ²SCIEX, Concord, ON

TOF am 09:10 **Ion-Ion Proton Transfer and Parallel Ion Parking for Top-Down Analysis of Complex Protein Mixtures;** Scott A Ugrin¹; Michelle A English¹; Dina L Bai¹; John E P Syka²; Jeffrey Shabanowitz¹; Donald F Hunt¹; ¹University of Virginia, Charlottesville, VA; ²Thermo Fisher Scientific, San Jose, CA

- TOF am 09:30 **System Architecture for Charge-independent Mass Spectrometry using Nanomechanical Resonators**; Shawn Fostner^{1,2}; Sergio Dominguez Medina^{1,3,4}; Marc Sansa Perna^{1,2}; Thomas Alava^{1,2}; Ann-Kathrin Stark^{1,3,4}; Ariel Brenac^{5,6}; Henri Blanc^{1,2}; Marc Gely^{1,2}; Sébastien Hentz^{1,2}; Christophe Masselon^{1,3,4}; ¹Université Grenoble Alpes, Grenoble, France; ²CEA, LETI, Grenoble, France; ³CEA BIG-BGE, Grenoble, France; ⁴INSERM U1038, Grenoble, France; ⁵Université Grenoble Alpes, INAC-SP2M, Grenoble, France; ⁶CEA, INAC-SP2M, Grenoble, France
- TOF am 09:50 **Dual-Polarity Ion Trap Mass Spectrometry: Dynamic Control and Monitoring of Gas-phase Ion-ion Reactions**; Muyi He¹; Dan Guo¹; You Jiang²; Xiong Xingchuang²; Zejian Huang²; Xiang Fang²; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, China; ²National Institute of Metrology, Beijing, China
- TOF am 10:10 **Quadrupole Wideband Isolation Directed by Ion Mobility Drift Separation for Analyzing Complex Protein Digests**; Bruce Wang¹; Ruwan T Kurulugama¹; George Stafford¹; John Fjeldsted¹; Joseph Roark¹; Frank Kuhlmann¹; Gregor Overney¹; ¹Agilent Technologies, Santa Clara, CA

**8:30-10:30 am TUESDAY
LIPIDS AND PROFILING
Ginger Milne (Vanderbilt University)
Hemisfair Ballroom 2, level 3**

- TOG am 08:30 **Enhanced Discrimination of Healthy Human Brain Tissue and Glioma using Positive and Negative Polarity Desorption Electrospray Ionization with Data Fusion**; Clint Miles Alfaro¹; Alan K Jarmusch²; Valentina Pirro²; Eyas M Hattab³; Aaron A Cohen-Gadol³; Graham R Cooks⁴; ¹Purdue University, Winston-Salem, NC; ²Purdue University, West Lafayette, IN; ³Indiana University School of Medicine, Indianapolis, IN; ⁴Purdue University, West Lafayette, IN
- TOG am 08:50 **A Novel Post-column Derivatization Method for Profiling "Diolome" using LC/MS/MS**; Jun Yang¹; Debin Wan¹; Chang Wang¹; Bruce D Hammock¹; ¹University of California, Davis, Davis, CA
- TOG am 09:10 **Separation and Characterisation of Human Meibum Lipids by Differential Ion Mobility Mass Spectrometry**; Sarah E Hancock¹; Peta Snikeris¹; Stephen J Blanksby²; Todd W Mitchell¹; ¹University of Wollongong, Wollongong, Australia; ²Queensland University of Technology, Brisbane, Australia
- TOG am 09:30 **Nitrated Fatty Acids: Biomarkers of Inflammation and Regulators of Redox Homeostasis**; Stacy Gelhaus Wendell¹; Bruce A Freeman¹; Franca Golin-Bisello¹; Gregory Buchan¹; Sonia Salvatore¹; Soma Jobbagy¹; Kara Hughan¹; Mark Gladwin¹; ¹University of Pittsburgh, Pittsburgh, PA
- TOG am 09:50 **Structure Elucidation of Omega-3 Fatty Acid Fish Oil Glycerolipid Dietary Supplements by Supercritical Fluid Chromatography Q-TOF-MS**; Sheher Mohsin¹; Gene S Hall²; Joe Hedrick³; ¹Agilent Technologies, Schaumburg, IL; ²Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, Piscataway, NJ; ³Agilent Technologies, Wilmington, DE
- TOG am 10:10 **Characterizing the Natural History of Acute Radiation Syndrome of the Gastrointestinal Tract: Combining High Mass and Spatial Resolution using MALDI-FTICR-MSI**; Claire

Louise Carter¹; Jace W Jones¹; Kim Hankey²; Ann M Farese³; Thomas J MacVittie²; Maureen A Kane¹; ¹University of Maryland, School of Pharmacy Baltimore, MD; ²University of Maryland School of Medicine, Baltimore, MD; ³University of Maryland Baltimore, Baltimore, USA

**8:30-10:30 am TUESDAY
NATIVE MS IN STRUCTURAL BIOLOGY
Alison E. Ashcroft (University of Leeds)
Hemisfair Ballroom 1, level 3**

- TOH am 08:30 **Accurate Determination of the Carbohydrate Content of Highly Heterogeneous Glycoproteins by Native Mass Spectrometry**; Guanbo Wang^{1,2}; Albert J. R. Heck^{1,2}; ¹Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, The Netherlands; ²Netherlands Proteomics Center, Utrecht, The Netherlands
- TOH am 08:50 **High-Confidence Models of Multiprotein Complexes from Ion Mobility-Mass Spectrometry Datasets: Frontiers in Model Generation and Assessment**; Joseph D Eschweiler¹; Aaron T. Frank¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- TOH am 09:10 **Structural Characterization of Missense Mutations using High Resolution Mass Spectrometry: The Parkinson's Related Protein DJ-1 Case Study**; Gili Ben-Nissan¹; Almog Chotiner²; Michal Sharon²; ¹Weizmann Institute of Science, Rehovot, Rehovot; ²Weizmann Institute of Science, Rehovot, Israel
- TOH am 09:30 **Characterization of a Nitrogenase Complex from Azotobacter Vinelandii in Gas Phase using Native Mass Spectrometry And Ion Mobility**; Monika Tokmina-Lukaszewska¹; Natasha Pence¹; Rhessa Ledbetter²; Stephen Keable¹; Sudipta Shaw²; Zhiyong Yang²; John Peters¹; Lance Seefeldt²; Brian Bothner¹; ¹MSU, Bozeman, MT, Bozeman, MT; ²Utah State University, Logan, UT
- TOH am 09:50 **Top Down Proteomics and Native Ion Mobility-MS Reveals Phosphorylation-Mediated Effects on NF-kB Conformation and Interactions**; Matthias Vonderach¹; Manohar Dange¹; Claire Evers¹; ¹University of Liverpool, Liverpool, United Kingdom
- TOH am 10:10 **Charge Detection Mass Spectrometry Monitors Virus Assembly from Single Subunit to Complete Capsid**; Corinne Lutomski¹; Kevin Zhao²; Adam Zlotnick²; Martin F Jarrold²; ¹Indiana University, Bloomington, IN; ²Indiana University, Bloomington, IN

**10:30 AM – 2:30 PM, TUESDAY
TUESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm**

**2:30-4:30 pm TUESDAY
ENVIRONMENTAL: NEW INSTRUMENTATION AND
APPROACHES**

**Alla Zelenyuk (Pacific Northwest National Laboratory)
Hall 1, level 1**

- TOA pm 02:30 **Comparison of Soft Ionisation Techniques for the High Resolution Mass Spectrometry Analysis of Environmental Samples with Complex Matrices;** Ivan Kourtshev¹; Pak Yiu Paddy Szeto¹; Duncan Scott¹; Ian P O'Connor²; Olalekan Popoola¹; Arthur Zielinski¹; John C Wenger²; Markus Kalberer¹; ¹University of Cambridge, Cambridge, UK; ²University College Cork, Cork, Ireland
- TOA pm 02:50 **Laser Diode Thermal Desorption (LDTD)-MS and Machine Learning: a Novel Approach for Ultra Fast Environmental Analysis;** Pier-Luc Plante^{1,2}; Prudencio Tossou¹; Alexandre Drouin¹; Francis Brochu¹; François Laviolette¹; Mario Marchand¹; Jacques Corbeil^{1,2}; ¹Université Laval, Québec, Canada; ²Centre de recherche du CHU de Québec, Québec, QC
- TOA pm 03:10 **Measurement of Protonated Ions as Sensitive Indicator for Neutral Polycyclic Aromatic Hydrocarbon Chemistry in Combustion by Time-of-Flight Mass Spectrometry;** Yasin Karakaya¹; Thomas Bierkandt¹; Tina Kasper¹; ¹Thermodynamics, University of Duisburg-Essen, Duisburg, Germany
- TOA pm 03:30 **Ultrafast Quantitative Analysis of Pesticides in Food and Environmental Matrices by SPME-Transmission Mode and Direct Analysis in Real Time;** Emanuela Gionfriddo¹; German Augusto Gomez-Rios¹; Justen Poole¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo ON, Canada
- TOA pm 03:50 **Multivariate Statistics Applied to MALDI-TOF MS Data of Pollen Samples;** Franziska Lauer^{1,2}; Stephan Seifert^{1,2}; Janina Kneipp^{1,2}; Steffen M. Weidner³; ¹Federal Institute f. Material Research and Testing, Berlin, Germany; ²Humboldt University, Berlin, Germany; ³Fed.Inst.f.Mat.Research, Berlin, Berlin
- TOA pm 04:10 **On the Application of Electrochemistry-Mass Spectrometry to Study the Biotransformation of UV Blockers in the Environment;** Pedro A. Segura¹; Delphine Canon¹; Emmanuel Eysseric¹; ¹Université de Sherbrooke, Sherbrooke, QC

**2:30-4:30 pm TUESDAY
NEW DEVELOPMENTS IN ION DETECTION**

**Martin F. Jarrold (Indiana University)
Room 221, level 2**

- TOB pm 02:30 **The Dynamics of Superconducting Tunnel Junction Cryodetector Energy Response as it Relates to Ion Structure, Surface Area and Density;** Logan D. Plath¹; David M Sipe¹; Jonathan Feldman¹; Chenjie Zeng¹; Yuxiang Chen¹; Rongchao Jin¹; Mark E. Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA
- TOB pm 02:50 **A Novel Charge Detection Rectilinear Ion Trap Mass Spectrometer (CD-RIT MS) for Detection of High Mass Proteins;** Avinash Adhikrao Patil¹; Szu-Wei Chou¹; Chen-Wei Lee¹; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng Hualien, Taiwan
- TOB pm 03:10 **Neutralization Charge Detection Method Facilitating Fast and Sensitive Hetero-Phase Ion Detection;** Ko-Keng Chang^{1,2}; Yi-Hong Cai¹; Yi-Sheng Wang¹; ¹Genomics Research Center, Academia Sinica Taipei, Taiwan; ²Chemistry Department, National Taiwan University, Taipei, Taiwan

- TOB pm 03:30 **Maximising Ion Detection Efficiency using Cycloidal Transport Of Secondary Electrons In Crossed Electric and Magnetic Fields;** Dick Stresau¹; Scott Morgan¹; Toby Shanley¹; ¹ETP Ion Detect, Clyde, Australia
- TOB pm 03:50 **A Novel Wide Dynamic Range oa-ToF Detection System Based on Dual 10-bit ADCs and FPGA Processing;** Martin Green¹; Garry Scott¹; Stephen Platt¹; Peter Spreadbury¹; Darrell Williams¹; Frank Buckley¹; Witold Niklewski¹; Stephen Hinde¹; Martin Palmer¹; John Chipperfield¹; ¹Waters, Wilmslow, United Kingdom
- TOB pm 04:10 **Multiple Frequency Resonance Methods in Quadrupole Ion Trap Mass Spectrometry: Expanding Capabilities and Improving Performance;** Dalton Snyder¹; Christopher Pulliam¹; Joshua S Wiley²; Jason Duncan³; R Graham Cooks¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²California Institute of Technology, Pasadena, CA; ³Acuity Brands Lighting Inc, Crawfordsville, IN

**2:30-4:30 pm TUESDAY
QUANTITATIVE ANALYSIS IN
DRUG DISCOVERY AND DEVELOPMENT**

**Jian Wang (Bristol-Myers Squibb)
Stars Ballroom 1, level 3**

- TOC pm 02:30 **The Potential of Micro Sampling in Regulated Bioanalysis using LC-MSMS;** Martijn Hilhorst¹; Roderik Prins²; Frank Schalken²; ¹PRA Health Sciences, Assen, Drenthe; ²PRA Health Sciences, Assen, The Netherlands
- TOC pm 02:50 **Universal LBA/LCMS Workflow for Protein Biotherapeutics PK Analysis in Preclinical Assay;** Bruce Aungst¹; Caroline Becker¹; Xun Wang¹; Lei Xiong²; Witold Woroniecki²; Yihan Li²; Suma Ramagiri²; Hua-fen Liu²; Zamas Lam¹; ¹QPS, Newark, DE; ²SCIEX, Redwood City, CA
- TOC pm 03:10 **A Trapping micro-LC/MS for Ultra-sensitive, Robust and High-Throughput Quantification of Biotherapeutics and Biomarkers in Complex Matrices;** Bo An¹; Ming Zhang¹; Yang Qu¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- TOC pm 03:30 **Measuring Drug-Target Engagement in Tissue Biopsies Using Affinity Extraction LC-MS/MS;** Eugene F. Ciccimaro¹; Yongxin Zhu²; Dmitry Ostanin²; Suzanne Suchard²; Jamus MacGuire²; Qing Xiao²; Ashok R Dongre²; Petia A Shipkova²; Timothy Olah²; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Princeton, NJ
- TOC pm 03:50 **A Label-free, Mass Spectrometry-based High Throughput Candidate Drug Screening Assay: Application to Smith-Lemli-Opitz Syndrome;** Jaqueline A Picache¹; Stephanie M Cologna^{2,1}; Alfred L Yergey¹; Pierre Picard³; Catherine Chen¹; Kathryn R Burkert¹; Christopher A Wassif¹; Wei Zheng¹; Forbes D Porter¹; ¹National Institutes of Health, Bethesda, MD; ²University of Illinois at Chicago, Chicago, IL; ³Phytronix Technologies, Quebec, Canada
- TOC pm 04:10 **Cleavable Antibody Drug Conjugate (ADC) Assay Support Enables ADC ADME and Discovery Programs;** Brian Rago¹; Fengping Li¹; Cong Wei¹; Xiaogang Han¹; Tracey Clark¹; Lindsay King¹; Nathan Tumey¹; Frank Barletta¹; Mauricio Leal¹; Steven Hansel¹; ¹Pfizer, Groton, CT



TUESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm TUESDAY ION MOBILITY, FAIMS & DMS: NEW DEVELOPMENTS & APPLICATIONS George Stafford (Agilent Technologies) Stars Ballroom 2-3, level 3

- TOD pm 02:30 **Moving beyond Collision Cross Sections: Using Cryogenic Infrared Spectroscopy to Determine the Structures of the Mobility-Selected Neuropeptide CabTRP1a (APSGFLGMR-NH2);** Michael Kamrath¹; Matthew Glover²; Marta A. S. Perez¹; Ursula Rothlisberger¹; David E Clemmer²; Thomas R Rizzo¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ²Indiana University Dept. Chemistry, Bloomington, IN
- TOD pm 02:50 **Integration of High-field Asymmetric Waveform Ion Mobility and Ambient Ionization Mass Spectrometry for Biological Tissue Imaging;** Clara Feider¹; Livia S. Eberlin²; ¹University of Texas at Austin, Austin, Texas; ²University of Texas at Austin, Austin, TX
- TOD pm 03:10 **A Theoretical and Empirical Approach to Separating Isomer Classes in Uniform Field Ion Mobility;** James Dodds¹; Jody C May¹; John A McLean¹; ¹Vanderbilt University, Nashville, TN
- TOD pm 03:30 **Separation and Identification of Isomeric Lipids using a Combination of Differential Mobility Spectrometry and Ozone-induced Dissociation;** Stephen J Blanksby¹; Berwyck L. J. Poad²; Alan T. Maccarone³; Todd W Mitchell³; ¹Queensland University of Technology, Brisbane, QLD; ²Queensland University of Technology, Brisbane, Australia; ³University of Wollongong, Wollongong, Australia
- TOD pm 03:50 **Gas Phase Epitope Mapping - A Mass Spectrometric Method for Accurate, Facile, and Rapid Identification of Specific Antibody-Peptide Reactivities;** Yelena Yefremova¹; Frimpong-Manso Kwabena Opuni¹; Hans-Juergen Thiesen²; Michael O Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²Institute of Immunology, Rostock, Germany
- TOD pm 04:10 **Ultrahigh IMS Resolution using Novel Traveling Wave Approaches and Long Serpentine Path Length SLIM Modules;** Richard D. Smith¹; Liulin Deng¹; Ahmed Hamid¹; Ian K Webb¹; Sandilya V.B. Garimella¹; Erin S Baker¹; Yehia M Ibrahim¹; ¹PNNL, Richland, WA

2:30-4:30 pm TUESDAY QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS Amber L. Mosley (Indiana University School of Medicine) Stars Ballroom 4, level 3

- TOE pm 02:30 **Disease-specific Post-translational Modifications in Cystic Fibrosis;** Sandra Pankow¹; Casimir Bamberger¹; John Yates¹; ¹The Scripps Research Institute, La Jolla, CA
- TOE pm 02:50 **PTM'omics: What Do We Learn from Surveying Many Modifications Simultaneously in Non-Enriched Proteomes? A Study of Lysine Acylations;** Hong Nguyen¹; Michael McInerney²; Robert Gunsalus¹; Joseph A Loo¹; Rachel Ogorzalek Loo¹; ¹UCLA, Los Angeles, CA; ²University of Oklahoma, Norman, OK
- TOE pm 03:10 **Redox Proteomics to Study Cysteine Status in Alzheimer's Disease;** Renā A. S. Robinson¹; Liqing Gu¹; ¹University of Pittsburgh, Pittsburgh, PA

- TOE pm 03:30 **The Phosphoproteome of the NCI-60 Cell Line Panel Reveals Markers of Drug Sensitivity;** Benjamin Ruprecht¹; Chen Meng²; Martin Frejno³; Alexander Hogrebe¹; Dominic Helm²; Bernhard Kuster²; ¹TU Muenchen, Freising, Germany; ²TU Muenchen, Freising, Germany; ³Oxford University, Oxford, United Kingdom
- TOE pm 03:50 **Identification of Histone ADP-Ribosylation Sites using High Resolution Mass Spectrometry;** Kelly Karch¹; Benjamin A. Garcia¹; Ben E. Black¹; ¹University of Pennsylvania, Philadelphia, PA
- TOE pm 04:10 **Comparative Ubiquitylome Analysis of Major Proteasome Inhibitors;** Tanya Rocio Porras-Yakushi¹; Michael Sweredoski¹; Sonja Hess¹; ¹Caltech, Pasadena, CA

2:30-4:30 pm TUESDAY IMAGING: COMPUTATIONAL METHODS AND ANALYSIS Theodore Alexandrov (EMBL / UCSD / SciLS) Hemisfair Ballroom 3, level 3

- TOF pm 02:30 **Absorption Mode Processing of MALDI-FT-ICR Imaging Data Improves Mapping of Gram-Negative Bacterial Virulence Factors on-Tissue;** Alison Scott¹; David P A Kilgour²; Robert K Ernst¹; David R Goodlett¹; ¹University of Maryland, Baltimore, MD; ²Nottingham Trent University, Nottingham, UK
- TOF pm 02:50 **Deep Autoencoders for Dimensionality Reduction of 3D Mass Spectrometry Imaging Data-Sets for Tumour Classification and Novel Subtypes Identification;** Paolo Inglese¹; James McKenzie¹; Anna Mróz¹; James Kinross¹; Elaine Holmes¹; Zoltan Takats¹; Jeremy K Nicholson¹; Robert C Glen^{1,2}; Kirill Veselkov¹; ¹Imperial College London, South Kensington Campus London, United Kingdom; ²University of Cambridge, Cambridge, UK
- TOF pm 03:10 **Dimensionality Reduction of MALDI Imaging Datasets using Non-Linear Redundant Wavelet Transform-based Representations;** Luis Mancera¹; Lyna Sellami²; Jamie Cunliffe²; Luis González¹; Omar Belgacem²; ¹Clover Bioanalytical Software, Granada, SPAIN; ²Shimadzu, Kratos Manchester, United Kingdom
- TOF pm 03:30 **Current Status and Applications of the Open Data Format imzML;** Nicolas Desbenoit¹; Amol Fatangare²; Andreas Roempp²; ¹Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; ²Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth
- TOF pm 03:50 **Generation of Realistic Synthetic Mass Spectrometry Imaging (MSI) Data for the Validation of Multivariate Analysis Methods;** Alexander Dexter^{1,2}; Alan Race²; Iain B Styles¹; Helen J Cooper¹; Josephine Bunch^{2,3}; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, Teddington, United Kingdom; ³University of Nottingham, Nottingham, UK
- TOF pm 04:10 **Characterisation of Molecular Signatures in the Xenograft Microenvironment using Novel Tools to Combine Histopathology and Mass Spectrometry Imaging Data;** Jo Cappell¹; Gert B Eijkel¹; Martha Ingola¹; Richard J A Goodwin²; Peter Webborn²; Ron M A Heeren¹; ¹M4I Institute - Maastricht University, Maastricht, The Netherlands; ²AstraZeneca, Cambridge, UK



2:30-4:30 pm TUESDAY
METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS
Nichole Reisdorph
(University of Colorado Anschutz Medical Campus)
Hemisfair Ballroom 2, level 3

- TOG pm 02:30 **Symbiotic Interaction between Legumes and Rhizobia Explored by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation;** Sylvia Stopka¹; Beverly Agtuca²; Christopher Anderton³; David W Koppenaal³; Ljiljana Pasa-Tolic³; Gary Stacey²; Akos Vertes¹; ¹George Washington University, Washington, District of Columbia; ²University of Missouri, Columbia, MO; ³Pacific Northwest National Laboratory, Richland, WA
- TOG pm 02:50 **Temporal Analysis of Living Human Bronchial Epithelial Cell Signaling and Drug Transportation using nano-DESI MS;** Ingela Lanekoff¹; Erik Lundin¹; Jan-Christer Ulvinge²; Mark Nicholas²; ¹Uppsala University, Uppsala, Sweden; ²AstraZeneca R&D, Gothenburg, Sweden
- TOG pm 03:10 **Solid Phase Microextraction as a Sample Preparation Tool for Untargeted Analysis of Brain Tissue;** Nathaly Reyes-Garces¹; Ezel Boyaci¹; German Augusto Gomez-Rios¹; Barbara Bojko¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo ON, Canada
- TOG pm 03:30 **AN Integrated Platform for Quantitative Full-Scan Polar LC/MS Metabolomics Reveals Structured Environmental Stress Response in the Yeast *Saccharomyces Cerevisiae*;** Amy Anne Caudy¹; Julia A Hanchard¹; Kaitlin U Lavery¹; Anton Lunyov¹; Olga Zaslaver¹; Soumaya Zlitni¹; Adam Rosebrock¹; ¹University of Toronto, Toronto ON, Canada
- TOG pm 03:50 **High-throughput Targeted Metabolomics of CoA Metabolites for Modulation of Antibiotic Influx and Efflux in Gram Negative Bacteria;** Christopher M. Rath¹; Bret Benton¹; Javier De Vicente²; Cindy Li¹; Bob Moreau¹; Xiaoyu Shen¹; Lisha Wang¹; Brian Feng¹; ¹Novartis Institutes for Biomedical Research, Emeryville, CA - California; ²Denali Therapeutics, South San Francisco, CA - California
- TOG pm 04:10 **Higher-throughput Annotation of Plant Metabolomes using Spectral Matching, Computational Identification Tools and Empirical UHPLC-MS-SPE-NMR;** Lloyd W. Sumner^{1,2}; Feng Qiu^{1,2}; Dennis Fine²; Daniel Wherritt³; Zhentian Lei¹; Aiko Barsch⁴; ¹University of Missouri, Columbia, MO; ²The Samuel Roberts Noble Foundation, Ardmore, OK; ³University of Texas, San Antonio, TX; ⁴Bruker Daltonics GmbH, Bremen, Germany

2:30-4:30 pm TUESDAY
PROTEIN-LIGAND INTERACTIONS
John S. Klassen (University of Alberta)
Hemisfair Ballroom 1, level 3

- TOH pm 02:30 **An Integrated HDX-MS-Based Platform Characterizes the Interaction between apoE3 and a ligand: High-Resolution Kinetics, PLIMSTEX, and SUPREX;** Hanliu Wang¹; Don L Rempel¹; Tridib Mondal²; Carl Frieden²; Michael L Gross¹; ¹Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO; ²Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St. Louis, MO
- TOH pm 02:50 **Ligand-Induced Disorder-to-Order Transitions Characterized by Structural Proteomics;** Nicholas I Brodie¹; Geoff M Gudavicius²; Christopher J Nelson²; Evgeniy V Petrotchenko¹; Christoph

H. Borchers^{3,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ³University of Victoria - Genome BC Proteomics Centre, Victoria, BC

- TOH pm 03:10 **Targeted MS-based Approach for Protein Ligand Binding Analysis in Complex Biological Mixtures using a Phenacylbromide Modification Strategy;** Lorain Jin¹; Carol H Ball²; Michael C Fitzgerald¹; ¹Duke University, Durham, NC; ²Agilent Technologies, Santa Clara, CA
- TOH pm 03:30 **Unveiling the Heterogeneity of an Uncharacterized Manganese Oxidizing Multicopper Oxidase Using High Resolution Native Mass Spectrometry and Surface Induced Dissociation;** Mowei Zhou¹; Jing Yan²; Christine Romano³; Yang Song²; Jeremy J Wolff⁴; Joshua Gilbert²; Randall E Pedder⁵; Bradley Tebo³; Vicki H Wysocki²; Ljiljana Pasa-Tolic¹; ¹Pacific Northwest National Laboratory - PNNL, Richland, WA; ²Ohio State University, Columbus, OH; ³Oregon Health & Science University, Portland, OR; ⁴Bruker Daltonics, Billerica, MA; ⁵Ardara Technologies L.P., Ardara, PA
- TOH pm 03:50 **Probing KIX:Peptide Allosteric Interactions by Ion Mobility-Mass Spectrometry;** Jessica Rabuck-Gibbons¹; Jean M Lodge¹; Anna K Mapp¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- TOH pm 04:10 **Tetrameric BanLec Neutralises HIV through Bidentate Binding to Specific Viral Glycan Structures;** Jonathan Hopper¹; Oliver Grant²; Stephen Ambrose¹; Stefanie Krumm³; Timothy Allison¹; Mark Tully⁴; Laura Pritchard¹; Gabriel Ozorowski⁵; Andrew Ward⁵; Max Crispin¹; Katie Doores³; Robert J Woods²; Justin Benesch¹; Carol V Robinson¹; Weston Struwe¹; ¹University of Oxford, Oxford, UK; ²University of Georgia, Athens, GA; ³King's College London, London, UK; ⁴Diamond Light Source, Didcot, UK; ⁵The Scripps Research Inst., La Jolla, CA

4:45 – 5:30 PM, TUESDAY AFTERNOON
AWARD LECTURE
Jenny Brodbelt (University of Texas, Austin) presiding
Hall 1, level 1

Presentation of the 2016 Research Awards



Biemann Medal

Kristina "Kicki" Håkansson
 University of Michigan

There are light refreshments in common areas.

01 Glycoproteomics: Site Specific Glycan Analysis
Ron Orlando presiding
Room 220, level 2

Modulating the activities and functions of proteins is a significant role of post-translational modifications (PTMs), with glycosylation being an excellent example. Glycan moieties of glycoproteins affect protein folding, stability, and localization and thus play a role in numerous biological functions, including cell signaling, adhesion, and communication. The analysis of released glycans has been a primary focus of glyco-analytical development over the past several years. However, these glycan centric analyses do not provide information on the glycans present at each glycosylation sites. Often the site occupancy is critical for biological activity. This behavior is clearly shown with therapeutic antibodies, where glycans located in the variable domain influence the serum clearance rate while glycans in constant domain affect the activity. The comprehensive characterization of protein glycosylation microheterogeneity entails the identification and quantitation of isomeric glycan occupancy of potentially all glycosylation sites on a protein, which is a significantly more difficult challenge than glycomic profiling. This workshop critical evaluation of state-of-the-art methods currently employed for enrichment and analysis at a glycoproteomic level.

02 Ion Mobility: How to Interpret the Data
(Ion Mobility MS Interest Group)

Erin Baker, Valerie Gabelica, and Stephen Valentine presiding
Room 221, level 2

Over the past decade, MS instrumentation featuring various forms of mobility-based separations have proliferated. One hurdle to intra- and inter-instrumental platform data comparison is, however, the lack of common interpretation schemes and practical tools. In part this results from gaps in knowledge related to correct data interpretation. This workshop will discuss the tools currently available for ion mobility data analyses, and participants will be invited to show tricky cases where data analysis can lead to ambiguous or erroneous interpretations. The workshop discussion will help make progress toward finding common ground and sound fundamental principles for the correct interpretation of ion mobility data.

03 H/D Exchange, Covalent Labeling & Cross-Linking
(H/D Exchange, Covalent Labeling & Cross-Linking Interest Group)

Joshua Sharp and David Weis presiding
Room 225A, level 2

This workshop will provide a forum for discussing hydrogen exchange, covalent labeling, and cross-linking approaches for protein analysis (structure, function, folding, dynamics). There will be a several brief presentations introducing late-breaking advances in MS-based methods, experiments, data analysis, and applications to the attendees. The goal of these abbreviated presentations will be to stimulate discussion. There will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

04 Food Safety & Security: HRMS Applications
(Flavor, Fragrance & Foodstuff Interest Group)
Walter Hammack and David Schroeder presiding
Room 225B, level 2

A continued discussion of applications and developments in the use of High Resolution Mass Spectrometry (HRMS) in food safety and food security. A focus on new developments and applications in pesticide residue analysis, non-target screening, and natural product authenticity.

05 Microcontrollers and Microcomputers:
Emerging Technologies
Vincent Sica and Bindesh Shrestha presiding
Room 225C, level 2

Smaller is becoming better - computers as smart phones, nanotechnology, miniature mass spectrometers, even tiny homes! The latest trend in "do-it-yourself" (DIY) electronics is microcontrollers (i.e. Arduino) and microcomputers (i.e. Raspberry Pi). These small, yet powerful devices have put electronic innovation right into our hands. Sensors, displays, and detectors can all be added at a whim without requiring the knowledge of advanced computer circuitry.

This year's discussion will focus on the implementation and use of microcontrollers and microcomputers to support advancements in the field of mass spectrometry. Short presentations showcasing applications of this technology will be followed by the discussion of the following topics:

- 1) Hardware (microcontrollers and microcomputers)
- 2) Software/code
- 3) Where to begin/which microelectronic is right for you?
- 3) Utility of DIY-microelectronics in mass spectrometry
- 4) Add-ons of the future (what type of sensors, displays, and detectors could really help push advancement in MS?)
- 5) Ideas (Active audience participation is encouraged to discuss new ideas/concepts/suggestions)

These discussions aim to not only educate others on how they can improve their research with microcontrollers and microcomputers, but also to spark ideas on what the future may bring to the growing technologies of both microelectronics and mass spectrometry.

06 DNA/RNA Adducts: Assay Development in
Detection and Quantification
(Oligonucleotides and Nucleic Acids Interest Group)
Patrick Limbach and Laixin Wang presiding
Room 225D, level 2

Recent mass spectrometry developments now enable high sensitivity detection of DNA or RNA adducts (or modifications). This workshop will focus on the practical issues involved in developing MS-friendly assays to measure these adducts. Selected presentations will illustrate assay development with a focus on sample prep, HPLC conditions, and data analysis. An emphasis in these informal discussions will be on pitfalls and "what did not work" to freely share strengths and weaknesses of assay development. The remaining time will be spent discussing challenges facing MS assays, especially given the advantages now being presented by high-throughput genome-based technologies.

07 Petroleum and Biofuels: Handling the Data (Energy,
Petroleum & Biofuels Interest Group)
Mark Barrow and Lateefah Stanford presiding
Room 301A, level 3

Petroleum-related mass spectra, often acquired using ultrahigh resolution instruments, are well-known for their complexity. With coupling of ion mobility and chromatography becoming more widespread, the level of complexity will be expected to significantly increase. Accompanying this, issues such as data size, data analysis, usage of chemometrics, software development, and comparisons of results from different analytical techniques will become progressively important. The workshop will highlight some of the existing approaches and will focus upon an active discussion of the current and emerging challenges.

08 Metabolism of Biotherapeutics: When, Why and How?
(DMPK Interest Group)
Kevin Bateman and Philip Tiller presiding
Room 301BC, level 3

Biotherapeutics are a steadily growing proportion of the pharmaceutical research and development landscape. Molecules are evolving beyond traditional monoclonal antibodies and antibody-drug conjugates

to include bispecifics, truncated mAbs, nanobodies, cyclic and stapled peptides, Ig fragments, Non-Ig based scaffolds and so on. Understanding the metabolism of these new modalities is an expanding opportunity for mass spectrometry and requires that traditional small molecule scientists adapt to these new large(r) molecules. The goal of this workshop is to stimulate a discussion on the when, why and how for the metabolism of biotherapeutics in the discovery, pre-clinical and clinical arena. A panel will offer opening comments on the current state and provide thoughts on where the field is going. Questions from the audience will be strongly encouraged to stimulate robust discussion.

09 Modification of Commercial Instruments for Fundamental Research (Fundamentals Interest Group)

**Alessandra Ferzoco and Michael Van Stipdonk presiding
Room 302A, level 3**

It was once the case that building instruments from scratch was essential for fundamental gas phase ion chemistry research. More recently it seems that the rather astounding performance of commercial instruments and increasing pressure for short project time frames has sparked a trend of modifying commercial instruments and working within academic/industrial collaborations. The purpose of the workshop is to explore the elements of effective instrument design within such collaborations. A variety of instruments that range in purpose and invasiveness of the modification will be presented, and both the researchers and company representatives will be present for discussion. We hope the workshop will provide guidance for researchers designing experiments and deciding where to be on the continuum between building from scratch and near-in-tact commercial instruments.

10 Lipidomics in the Era of Systems Biology: The Big Fat Challenges (Lipids and Lipidomics Interest Group)

**Christer Ejssing and Todd Mitchell presiding
Room 302BC, level 3**

There is a growing interest in using lipidomics for systems biology studies for understanding the molecular underpinnings of cellular processes and mechanisms of diseases. This workshop will focus on key challenges in integrating lipidomics with other -omics technologies, and how computational strategies can be designed to support meaningful insights into (patho)physiological processes. The discussion will be led by a panel of experts who will invite opinion from participants on current solutions and challenges in using lipidomics for systems biology studies of lipid function in both basic and clinical sciences.

11 Undergraduate Research in Mass Spectrometry (Undergraduate Research in MS Interest Group)

**Elaine Marzluff and Megan Gessel presiding
Room 303A, level 3**

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research experiences into successful scientific careers. Panelists will discuss their experiences applying to graduate school and transitioning to a graduate school research environment, as well as working in industrial labs.

12 The Chorus Project: Sustainable Cloud Solution for MS Data

**Michael MacCoss, Andrey Bondarenko, Christine Wu, and Nathan Yates presiding
Room 303BC, level 3**

The storage, sharing, analysis, and public dissemination of mass spectrometry data is a major challenge for our community. The lack of permanent infrastructure and sustainability is clearly exemplified by the discontinuation of noted resources such as Tranche, NCBI Peptidome, and more recently, the NHGRI's announcement that the funding for many key data resources are in jeopardy. Chorus provides the framework to facilitate a community supported solution to big data generated by the mass spectrometry field. Chorus is a professionally developed application that has a graphical user interface targeted towards the organization and visualization of mass spectrometry data stored on the Amazon cloud. Uploaded data can be exclusive and

private, shared with a specified group of collaborators, or made entirely public. Software tools can be added through a software developer's kit. These tools provide analytical workflows and can be made accessible to the community. Our recent focus has been the integration of analytical workflows such as Byonic, Comet, MaxQuant, PeakExplorer, Pecan, and Skyline.

13 Data Independent Acquisition (Data Independent Acquisition Interest Group)

**Ludovic Gillet and Jarrett Egerton presiding
Room 304, level 3**

Data independent acquisition (DIA) is a versatile mass spectrometry approach that aims to comprehensively record time-resolved fragment ion (MS/MS) signals for all detectable analytes in a sample. To identify and quantify analytes from those complex time- and mass-continuous MS/MS data structures, a diverse panel of analysis strategies is now available. These include leveraging spectral libraries, adapting DIA data for traditional database search engines, redesigning search engines to handle highly chimeric spectra, and detecting peptides/analytes based on extracted chromatograms. Notably, some strategies begin with a collection of features derived from the data (e.g. individual spectra, groups of spectra, or co-eluting peaks) and aim to interpret those features to generate identifications. Other strategies begin with a collection of analytes (e.g. a list of peptides) and query the data for evidence of detection. Each strategy can also differ in the modeling of a decoy scoring distribution and ultimately the assessment of false discovery rate. This workshop aims to disentangle the wealth of DIA analysis strategies available, to discuss the advantages and disadvantages of each approach, and to propose the adoption of a consensus nomenclature to meaningfully refer to them in future DIA studies.

14 Good Manufacturing Practice (GMP); Mass Spectrometric Instrument Qualification

**Gyorgy Vas presiding
Room 305, level 3**

This workshop will focus on initiating a discussion between the instrument users, regulators and the instrument vendors, to discuss issues relating to regulatory compliance. More rigorous regulatory expectations are requiring higher instrument qualification standards and more involved calibration processes. This workshop is intended to discuss best practice approaches and potential qualification issues.

**AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL**

8:30-10:30 am WEDNESDAY
ENERGY, PETROLEUM AND BIOFUELS: STRUCTURE, QUANTIFICATION, AND DATA ANALYSIS
Patrick G. Hatcher (Old Dominion University)
Hall 1, level 1

- WOA am 08:30 **In ESI-source H/D Exchange Facilitated a Structural Characterization of Individual Compound in Complex Mixtures by FTICR MS;** Alexey S Kononikhin^{1,2}; Yuri Kostyukovich³; Alexander Zhrebek⁴; Igor A Popov^{1,5}; Oleg N Kharybin^{2,6}; Evgeny Kukaev^{1,5}; Andrey Konstantinov⁴; Irina V Perminova⁴; Eugene Nikolaev^{1,2,5,6,7}; ¹*Moscow Institute of Physics and Technology, Moscow, Russia*; ²*Institute for Energy Problems of Chemical Physics, Moscow, Russia*; ³*Skolkovo Institute of Science and Technology, Skolkovo, Russia*; ⁴*Lomonosov Moscow State University, Moscow, Russia*; ⁵*Emanuel Institute of Biochemical Physics, Moscow, Russia*; ⁶*Institute of Biomedical Problems RAS, Moscow, Russia*; ⁷*Skolkovo Institute of Technology, Moscow, Russia*
- WOA am 08:50 **Characterization of Organic Indicator Compounds of Petroleum Biosourcing using Novel Soft Ionization and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Jeremy Nowak¹; Robin Weber¹; Pravin Shrestha¹; Dana Loutey¹; Amy McKenna²; John Coates¹; Allen Goldstein¹; ¹*UC Berkeley, Berkeley, California*; ²*National High Magnetic Field Laboratory, Tallahassee, FL*
- WOA am 09:10 **High-resolution Broad Mass Range Collision-Energy Scanning Tandem Mass Spectrometry for Structural Characterization of Asphaltene Molecular Ions;** Xueming Dong¹; Xin Lu²; Yuyang Zhang¹; Weijuan Tang^{3,1}; Hilkka Kenttamaa¹; ¹*Purdue University, West Lafayette, IN*; ²*Harbin Institute of Technology, Harbin, China*; ³*Dow AgroSciences, Indianapolis, IN*
- WOA am 09:30 **Multidimensional Comprehensive Gas Chromatography with High Resolution-TOFMS/photo Ionization-TOFMS: Combining Ultra-high Chromatographic Resolution, Accurate Mass-information and Soft Photoionisation for Petrochemical Samples;** Thomas Groeger¹; Maximilian Jennerwein²; Benedikt Weggler¹; Mohammad Saraji-Bozorgzad³; Juergen Wendt⁴; Ralf Zimmermann⁵; ¹*Helmholtz Zentrum Muenchen, Oberschleissheim, Germany*; ²*ASG GmbH, Augsburg, Germany*; ³*Photonion GmbH, Schwerin, Germany*; ⁴*LECO Instrumente GmbH, Moenchengladbach, Germany*; ⁵*University of Rostock, Rostock*
- WOA am 09:50 **Reaction Pathway Analysis using Isotopically-Labeled Glucose in Real-Time Monitoring of Thin-Film Fast Pyrolysis;** Carolyn Hutchinson¹; Kristen O'Connor¹; Young Jin Lee¹; ¹*Iowa State University, Ames, IA*
- WOA am 10:10 **UPLC-MS and MS/MS of Grass Lignins: Evidence for New Structural Units and Cross-Linkers;** Afrand Kamali Sarvestani^{1,2}; Leonardo Da Costa Sousa^{3,4}; Venkatesh Balan^{3,4}; Xiaoxiao Liu¹; Bruce Dale^{3,4}; A Daniel Jones III^{1,2,5}; ¹*Department of Chemistry, Michigan State University, East Lansing, MI*; ²*DOE Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI*; ³*Department of Chemical Engineering and Material Science, Michigan State University, East Lansing, MI*; ⁴*DOE Great Lake Bioenergy Research Center, Michigan State University, East Lansing, MI*; ⁵*Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*

8:30-10:30 am WEDNESDAY
FUNDAMENTALS: ENERGETICS AND MECHANISMS OF UNI AND BIMOLECULAR REACTIONS
John R. Stutzman (The Dow Chemical Company)
Room 221, level 2

- WOB am 08:30 **Mechanistic Study of Gas Phase In-source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-ESI/Tandem Mass Spectrometry;** Huaming Sheng¹; Rong-Sheng Yang¹; Katrina M Lexa¹; Edward Sherer¹; Li-Kang Zhang¹; Bangping Xiang¹; Roy Helmy¹; ¹*Merck, Darmstadt, Germany*
- WOB am 08:50 **Probing the Effect of Charge on the Energetics and Reactivity of Distonic Peroxyl Radical Ions in the Gas Phase;** Peggy Williams¹; Nadia Skeljo¹; David Marshall¹; Benjamin Kirk²; Berwyck Poad^{1,3}; Stephen Blanksby¹; ¹*Queensland University of Technology, Brisbane, Australia*; ²*Lawrence Berkeley Nat'l Lab, Berkeley, CA*; ³*University of Wollongong, Wollongong, Australia*
- WOB am 09:10 **Computational and Experimental Investigation of Gas Phase Ion/Ion Reactions between Nucleophiles and HOAt/HOBt Reagents;** Jiexun Bu¹; Feifei Zhao¹; Scott A McLuckey¹; ¹*Purdue University, West Lafayette, IN*
- WOB am 09:30 **Photo-Electron Transfer Dissociation Pathways Reveal Zwitterion Locations in Peptides;** Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- WOB am 09:50 **Reactions of Hydroxyl Radicals and Cysteine Disulfide Derivatives (CySSR) – Mechanism and Reactivity Studies;** Sarju Adhikari¹; M. Anglada Josep²; Joseph S. Francisco³; Yu Xia⁴; ¹*Purdue University, West Lafayette, IN*; ²*Institute of Advanced Chemistry of Catalonia, Barcelona, Spain*; ³*University of Nebraska-Lincoln, Lincoln, NE*; ⁴*Purdue University-Department of Chemistry, West Lafayette, IN*
- WOB am 10:10 **Radical-Mediated Peptide Tyrosine Nitration In Vacuo: Experimental Evidence and Theoretical Examination;** Ivan K. Chu¹; Cheuk Kuen Lai²; Wai Kit Tang³; Chi-Kit Siu³; ¹*University of Hong Kong, Hong Kong, China*; ²*The University of Hong Kong, Hong Kong, China*; ³*City University, Hong Kong, Hong Kong*

8:30-10:30 am WEDNESDAY
IMAGING: PHARMACEUTICALS AND METABOLITES
Livia D. Eberlin (University of Texas at Austin)
Stars Ballroom 1, level 3

- WOC am 08:30 **C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells;** Anna N Bloom¹; Hua Tian¹; Nicholas Winograd¹; ¹*Pennsylvania State University, University Park, PA*
- WOC am 08:50 **Spatio-temporal Metabolomics of Tumor Organoids Treated with Chloroquine;** Andrew Palmer¹; Eric Weaver²; Katherine A Kellersberger³; Amanda B Hummon²; Theodore Alexandrov¹; ¹*EMBL Heidelberg, Heidelberg, Germany*; ²*University of Notre Dame, Notre Dame, Indiana*; ³*Bruker Daltonic, Billerica, MA*
- WOC am 09:10 **Mass Spectrometry Imaging for Characterizing Parasite Host Interactions in Malaria Research;** Saleh Mahmud Khalil¹; Andreas Römpf¹; Jette Pretzel²; Katja Becker²; Bernhard Spengler¹; ¹*Institute of Inorganic and Analytical Chemistry, Justus Liebig University, Giessen, Hessen, Germany*; ²*Biochemistry and Molecular Biology, Institute of Nutritional Sciences, Justus Liebig University, Giessen, Hessen, Germany*

- WOC am 09:30 **Simultaneous Desorption Electrospray Ionization Mass Spectrometry Imaging of Multiple Neurotransmitters and Neuroactive Substances**; Mohammadreza Shariatgorji¹; Nicole Strittmatter²; [Anna Nilsson](#)³; Theodosia Vallianatou¹; Per Svenningsson⁴; Richard J A Goodwin²; Per E Andren¹; ¹*Uppsala University, Uppsala, Sweden*; ²*AstraZeneca, Cambridge, UK*; ³*Uppsala University, Uppsala*; ⁴*Karolinska Institute, Stockholm, Sweden*
- WOC am 09:50 **Visualizing Tumors in Three Dimensions: a First Look at Drug Distribution in Brain Tumors using 3D MSI**; David Calligaris¹; Armen Changelian¹; Katherine A Kellersberger²; Yonatan Morocz¹; Forest White³; Jeffrey N Agar⁴; Jann N Sarkaria⁵; Nathalie Y. R. Agar¹; ¹*Department of Neurosurgery, and Department of Radiology, BWH, and Department of Cancer Biology, Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA*; ²*Bruker Daltonics, Billerica, MA*; ³*Massachusetts Institute of Technology, Boston, MA*; ⁴*Department of Chemistry and Pharmaceutical Sciences, Northeastern University, Boston, MA*; ⁵*Department of Radiation Oncology, Mayo Clinic, Rochester, MN*
- WOC am 10:10 **Growth, Metabolism, and Antibiotic Susceptibility of Bacterial Colonies Imaged by Laser Ablation Electrospray Ionization Mass Spectrometry**; [Hang Li](#)¹; Pranav Balan²; Akos Vertes¹; ¹*George Washington University, Washington, DC*; ²*Thomas Jefferson High School for Science and Technology, Alexandria, VA*

**8:30-10:30 am WEDNESDAY
INSTRUMENTATION: MINIATURIZATION OF MS
Christopher C. Mulligan (Illinois State University)
Stars Ballroom 2-3, level 3**

- WOD am 08:30 **Development of a Point-of-Care (POC) Miniature Mass Spectrometry System**; [Xiao Wang](#)¹; Yue Ren¹; Li Linfan¹; Xinwei Liu²; Zheng Ouyang^{1,2}; ¹*Purdue University, West Lafayette, IN*; ²*Tsinghua University, Beijing, China*
- WOD am 08:50 **LITMS: Dual Ion Source Switchable Polarity Linear Ion Trap Mass Spectrometer for Space Flight Applications**; [Andrej Grubisic](#)^{1,2}; William B Brinckerhoff²; Friso Van Amerom³; Ryan Danell⁴; Veronica T Pinnick⁵; Ricardo Arevalo²; Xiang Li⁵; Stephanie Getty²; Daniel Glavin²; Lars Hovmand⁶; Phil Chu⁷; Kris Zacny⁷; Steve Rogacki⁸; Timothy J Cornish⁹; Paul Mahaffy²; ¹*University of Maryland, College Park, MD*; ²*NASA GSFC, Greenbelt, MD*; ³*Mini-Mass Consulting, Inc., Hyattsville, MD*; ⁴*Danell Consulting, Inc. Winterville, NC*; ⁵*University of Maryland, Baltimore County Greenbelt, MD*; ⁶*Linear Labs LLC, Washington DC, DC*; ⁷*Honeybee Robotics, Pasadena, CA*; ⁸*University of Michigan, Ann Arbor, MI*; ⁹*C&E Research, Inc. Columbia, MD*
- WOD am 09:10 **Reverse Gas Stack Model for Localization of Chemical Interests Utilizing Mobile Mass Spectrometry**; [Phillip Mach](#)¹; Kenneth C Wright²; Guido F Verbeck¹; ¹*University of North Texas, Denton, TX*; ²*Inficon, Syracuse, NY*
- WOD am 09:30 **miniSPLAT: A Miniaturized Aircraft-Compatible Single Particle Mass Spectrometer for in-situ Quantitative Multidimensional Single Particle Characterization**; [Alla Zelenyuk](#)¹; Dan Imre²; Jacqueline Wilson¹; David Bell¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Imre Consulting, Richland, WA*

- WOD am 09:50 **Development and Applications of Microchip Capillary Electrophoresis Coupled with High Pressure Mass Spectrometry**; [William McKay Gilliland](#)¹; John Michael Ramsey¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, NC*
- WOD am 10:10 **Multi-sample Reaction Monitoring: a Miniature Process Analytical Tool using a Miniature Ion Trap**; [Christopher J Pulliam](#)¹; Ryan M Bain¹; Heather I. Osswald¹; Dalton T Snyder¹; Stephen Ayrton¹; Shannon Raab¹; R. Graham Cooks¹; ¹*Purdue University, West Lafayette, IN*

**8:30-10:30 am WEDNESDAY
BIOMARKERS: QUALITATIVE ANALYSIS
Jennifer Van Eyk (Cedars-Sinai Medical Center)
Stars Ballroom 4, level 3**

- WOE am 08:30 **Organismal Level Dynamic Molecular Map of Mouse Proteome**; [Bingyun Sun](#)¹; Shizhen Qin²; Cynthia Lorang²; Gray Li²; Zhiyuan Hu²; Ken Liu³; Leory Hood²; ¹*Simon Fraser University, Burnaby, BC*; ²*Institute for Systems Biology, Seattle, WA*; ³*Simon Fraser University, Burnaby, BC, Canada*
- WOE am 08:50 **Intact Metabolome Analysis of Mice Biological Tissues by Probe Electrospray Ionization-Tandem Mass Spectrometry and Its Preliminary Application to Real-Time Analysis**; [Kei Zaitso](#)¹; Yumi Hayashi¹; Tasuku Murata²; Hiroki Nakajima²; Tetsuya Ishikawa¹; Maiko Kusano¹; Hitoshi Tsuchihashi¹; Akira Ishii¹; ¹*Nagoya University Graduate School of Medicine, Nagoya, Japan*; ²*Global Application Development Center, Shimadzu Corporation, Kyoto, Japan*
- WOE am 09:10 **Imaging Mass Spectrometry Identifies New Markers in Prostate Cancer Pathology**; [Kristina Schwamborn](#)¹; Peter Wild²; Jeremy L Norris³; Richard M Caprioli³; ¹*Technical University Munich, Munich*; ²*Institute of Surgical Pathology, University Hospital Zurich, Zurich, Switzerland*; ³*Department of Biochemistry and the Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*
- WOE am 09:30 **Top-down Proteomics Identified Novel Biomarkers for Hypertrophic Cardiomyopathy**; [Wenxuan Cai](#)¹; Zachery Gregorich¹; Andrew Messer²; Ziqing Lin¹; Zachary Hite¹; Steve Marston²; Takushi Kohmoto¹; Ying Ge¹; ¹*University of Wisconsin-Madison, Madison, WI*; ²*Imperial College London, London, UK*
- WOE am 09:50 **Profiling of Intact Proteins in the CSF of Alzheimer's Disease Patients using Top Down Proteomics: Revealing Specific Isoform Biomarker Candidates**; [Jerôme Vialaret](#)¹; Schmit Pierre-Olivier²; Audrey Gabelle³; Christophe Hirtz¹; Sylvain Lehmann¹; ¹*LBPC-IRB, CHU de Montpellier Montpellier, France*; ²*Bruker Daltonique S.A., Wissembourg, bas-rhin*; ³*Centre Mémoire Ressources Recherche, Montpellier, France*
- WOE am 10:10 **A Mass Spectrometry Approach to Discover Naturally-occurring Oxidation-specific Malondialdehyde Adducts**; [Juliane Weißer](#)¹; Christoph J Binder^{1,2}; Keiryn L Bennett¹; ¹*CeMM Research Center for Molecular Medicine, Vienna, Austria*; ²*Medical University of Vienna, Vienna, Austria*

8:30-10:30 am WEDNESDAY
INFORMATICS: MULTIMICS INTEGRATION AND
APPLICATION

Catherine Minogue (Hartwick College)
Hemisfair Ballroom 3, level 3

- WOF am 08:30 **Integrating and Mining Spatial Omics through Imaging Mass Spectrometry and Anatomical Atlases**; Nico Verbeeck¹; Jeffrey Spraggins²; Junhai Yang²; Etienne Waelkens^{3,4}; Richard M. Caprioli²; Raf Van de Plas¹; ¹*Delft University of Technology, Delft, The Netherlands*; ²*Vanderbilt University, Nashville, TN*; ³*KU Leuven, Leuven, Belgium*; ⁴*Sybioma, Leuven, Belgium*
- WOF am 08:50 **Mitochondrial Protein Functions Revealed by Global Mass Spectrometry Profiling**; Jonathan A Stefely^{1,2}; Nicholas W Kwiecien¹; Alexander S Hebert¹; Alicia L Richards¹; Elyse C Freiburger¹; Matthew J P Rush¹; Arne Ulbrich¹; Adam Jochem¹; Michael T Veling¹; Paul D Hutchins¹; Harald Marx¹; Michael S Westphall¹; David J Pagliarini^{1,2}; Joshua J Coon¹; ¹*University of Wisconsin Madison, Madison, Wisconsin*; ²*Morgridge Institute for Research, Madison, Wisconsin*
- WOF am 09:10 **Incorporating Multiple Information Layers to Understand Viral Antigen Presentation: Stepping Away from the Streetlamp**; Kavya Swaminathan¹; Peder J Lund¹; Caleb D Marceau¹; Niclas E Olsson¹; Mark M Davis¹; Jan Carette¹; Joshua E Elias¹; ¹*Stanford University, Stanford, CA*
- WOF am 09:30 **Quantitative Proteogenomics for Personalised Molecular Profiling**; Christoph Schlaffner¹; ²Theodoros Roumeliotis¹; Hendrik Weisser¹; James Wright¹; Jonathan Mudge³; Sergio Santos⁴; Graham Ritchie^{4,5,6,7}; Julia Steinberg⁵; Andreas Bender²; Alvis Brazma⁴; Jennifer Harrow³; Christine Le Maitre⁸; Mark Wilkinson⁹; Eleftheria Zeggini⁵; Jyoti Choudhary¹; ¹*Proteomic Mass Spectrometry, Wellcome Trust Sanger Institute, Cambridge, UK*; ²*Department of Chemistry, University of Cambridge, Cambridge, UK*; ³*Human and Vertebrate Analysis and Annotation Team, Wellcome Trust Sanger Institute, Cambridge, UK*; ⁴*European Bioinformatics Institute, European Molecular Biology Laboratory, Cambridge, UK*; ⁵*Department of Human Genetics, Wellcome Trust Sanger Institute, Cambridge, UK*; ⁶*Usher Institute of Population Health Sciences & Informatics, University of Edinburgh, Edinburgh, UK*; ⁷*MRC Institute of Genetics & Molecular Medicine, University of Edinburgh, Edinburgh, UK*; ⁸*Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, UK*; ⁹*Department of Human Metabolism, University of Sheffield, Sheffield, UK*
- WOF am 09:50 **Integrated Analysis of Human Tissues with a Multi-Omics Approach**; Hannes Hahne¹; ²Dongxue Wang²; Björn Hallström³; Lihua Li²; Anna Asplund⁴; Mathias Wilhelm^{1,2}; Harald Marx⁵; Frederik Ponten⁴; Mathias Uhlen³; Bernhard Kuster²; ¹*OmicsScouts GmbH, Freising, Germany*; ²*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*; ³*KTH Royal Institute of Technology, Stockholm, Sweden*; ⁴*Uppsala University, Uppsala, Sweden*; ⁵*University Wisconsin-Madison, Madison*
- WOF am 10:10 **Integration of Multiple 'Omics' Data Sets via Application of OnPLS Methodology**; Johan Trygg¹; Izabella Surowiec¹; ¹*Computational Life Science Cluster (CLiC), Umeå University, Umeå, Sweden*

8:30-10:30 am WEDNESDAY
MS IN THE QC LAB
Da Ren (Amgen)

Hemisfair Ballroom 2, level 3

- WOG am 08:30 **Application of Mass Spectrometry in the Quality Control Related Investigations During Protein Therapeutics Manufacturing and Stability Studies**; Li Tao; *Bristol-Myers Squibb Co., New Hope, PA*
- WOG am 08:50 **Monitoring Product Attributes in Biopharmaceutical Development and QC with LC/HRMS**; Scott Berger¹; Liuxi Chen¹; Min Du¹; Henry Y Shion¹; Ying-Qing Yu¹; ¹*Waters Corporation, Milford, MA*
- WOG am 09:10 **Extending the Capabilities of a MS Based Multi Attribute Characterization Method to Promote Quality by Design In Biotherapeutic Drugs**; Michael Blank¹; Jonathan L Josephs¹; Richard Rogers²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Just Biotherapeutics, Seattle, WA*
- WOG am 09:30 **Development of QC-Friendly Mass Spec Assay for Monitoring Antibody Oxidation**; Izabela Sokolowska¹; Jingjie Mo¹; Jia Dong¹; Michael J Lewis¹; Ping Hu¹; ¹*Janssen Research & Development, Malvern, PA*
- WOG am 09:50 **O-linked Glycosylation for a Fc Fusion Protein: Characterization and Understanding of Biological Relevance**; Le Zhang¹; Wael Hamouda¹; Joshua Pearson¹; Xiaoyan Guan¹; Hyo Chung¹; Jette Wypych¹; ¹*Amgen, Inc., Thousand Oaks, CA*
- WOG am 10:10 **Practical Applications of Mass Spectrometry in a Quality Control Laboratory**; Patrick Bulau; *Roche Diagnostics GmbH, Penzberg, Germany*

8:30-10:30 am WEDNESDAY
MACROMOLECULAR COMPLEXES

Mowei Zhou (Pacific Northwest National Laboratory)
Hemisfair Ballroom 1, level 3

- WOH am 08:30 **A Native Proteomics Platform for Untargeted Identification and Characterization of Protein Complexes**; Owen Skinner¹; Rafael Melani¹; Luca Fornelli¹; Nicole Haverland¹; Luis Henrique Ferrer Do Vale¹; Henrique Seckler¹; Peter Doubleday¹; Luis Schachner¹; Neil L Kelleher¹; Compton Philip¹; ¹*Northwestern University, Evanston, IL*
- WOH am 08:50 **Towards Routine Native Mass Spectrometric Analysis of Affinity-Isolated Endogenous Protein Complexes**; Paul Dominic B. Olinares¹; Amelia D Dunn¹; Julio C Padovan¹; Javier Fernandez-Martinez¹; Michael P Rout¹; Brian T Chait¹; ¹*The Rockefeller University, New York, NY*
- WOH am 09:10 **Integrating Native MS, Crosslinking-MS and HDX-MS with High-Resolution Cryo-Electron Microscopy Reveals the Molecular Architecture of the Sub-Megadalton Circadian Oscillator KaiCBA**; Philip Lössl¹; Joost Snijder^{1,2,3}; Jan Michael Schuller⁴; Anika Wiegand⁵; Ilka M Axmann⁵; Jürgen M Plitzko⁴; Friedrich Förster⁴; Albert J R Heck^{1,2}; ¹*Utrecht University, Utrecht, The Netherlands*; ²*Netherlands Proteomics Center, Utrecht, The Netherlands*; ³*University of Washington, Seattle, WA*; ⁴*Max Planck Institute for Biochemistry, Martinsried, Germany*; ⁵*Heinrich Heine University, Düsseldorf, Germany*
- WOH am 09:30 **Mobile-Proton MD Simulations for Modeling the Dissociation of Electrosprayed Protein Complexes**; Vlad Popa¹; Danielle Trecroce¹; Robert G McAllister¹; Lars Konermann¹; ¹*University of Western Ontario, London, Canada*

- WOH am 09:50 **Confirmation of Subunit-Subunit Connectivity and Topology of Computationally Designed Protein Complexes using Surface Induced Dissociation/Ion Mobility; Aniruddha Sahasrabudde¹; Yang Hsia²; Florian Busch¹; David Baker²; Vicki Wysocki¹; ¹The Ohio State University, Columbus, OH; ²University of Washington, Seattle, WA**
- WOH am 10:10 **Native Top-Down IRMPD of Macromolecular Protein Complexes — Game Over or Game Changing?; Huilin Li¹; Shirin Jamshidi²; Hong Hanh Nguyen¹; Iain Campuzano³; Rachel O Loo¹; Joseph A Loo¹; ¹UCLA, Los Angeles, CA; ²University of Warwick, Coventry, United Kingdom; ³Amgen, Inc., Thousand Oaks, CA**

**10:30 AM – 2:30 PM, WEDNESDAY
WEDNESDAY POSTER SESSION
Poster/Exhibit Hall**

Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

WEDNESDAY AFTERNOON ORAL SESSIONS

**2:30-4:30 pm WEDNESDAY
EXPOSOMICS: TARGETED, UNTARGETED AND
BIOINFORMATICS METHODOLOGIES**

**David M. Balshaw (National Institute of Environmental Health Sciences, National Institutes of Health)
Hall 1, level 1**

- WOA pm 02:30 **Causal Biomarker Discovery of Childhood Leukemia by Untargeted Metabolomics of Neonatal Dried Blood Spots; Lauren Petrick¹; William MB Edmands¹; Courtney L Schiffman¹; Alan Hubbard¹; Stephen M Rappaport¹; ¹UC Berkeley, Berkeley, CA**
- WOA pm 02:50 **High-coverage Metabolomic Analysis of Microliter Blood Using Isotope Labeling and High-resolution LC-MS; Wei Han¹; Liang Li¹; ¹Department of Chemistry, University of Alberta, Edmonton, AB, Canada**
- WOA pm 03:10 **Improving Detection and Coverage of Microbially-derived Metabolites using GC-MS Based Strategies for Targeted and Untargeted Profiling; Bhavapriya Vaitheesvaran¹; Vladimir Yong¹; Anthony Macherone²; Justin R Cross¹; ¹Memorial Sloan Kettering Cancer Center, New York, NY; ²Agilent Technologies, Little Falls, DE**
- WOA pm 03:30 **Novel Metabolites Revealed by High Resolution Orbitrap Mass Spectrometry and Their Implications in Quantitation of Urinary Exposure Markers; Jen-Yi Hsu¹; Jing-Fang Hsu¹; Yi-Jen Chen¹; Pao-Chi Liao¹; ¹National Cheng Kung University, Tainan, Taiwan**
- WOA pm 03:50 **An Exposomic Study of Health Assessment of Children with Autism and Control Children Using New Mass Spectrometry Methods for Quantitation; H.M Skip Kingston¹; Scott Faber²; Patrick benecewicz¹; ¹Duquesne University, Pittsburgh, PA; ²The children Institute, Pittsburgh, PA**
- WOA pm 04:10 **Detection and Identification of Generally Unknown Toxins and Altered Endogenous Components in Poisoned Patients using Data-Independent Acquisition and Untargeted Metabolomics; Cheng Chen¹; Ziquan Fan²; Xiaojie Tan²; Hui Xu³; Hongliang Jiang¹; Mingshe Zhu⁴; ¹Huazhong University of Science and Technology,**

Wuhan, China; ²Waters Technology (Shanghai) Co., Ltd, Shanghai, China; ³Maternal and Child Health Hospital of Hubei Province, Wuhan, China; ⁴Bristol-Myers Squibb, Princeton, NJ

**2:30-4:30 pm WEDNESDAY
FUNDAMENTALS: MOLECULAR MODELING AND QUANTUM MECHANICAL CALCULATIONS IN IM AND MS**

**Iain D. G. Campuzano (Amgen)
Room 221, level 2**

- WOB pm 02:30 **Molecular Dynamics/Kinetic Theory Algorithm for Numerical Determination of Electrical Mobility; Carlos Larriba Andaluz¹; Indiana University-Purdue University Indianapolis, Indianapolis, IN**
- WOB pm 02:50 **Using Molecular Dynamics Simulations to Uncover the Mechanism of Supercharging in Protein ESI; Lars Konermann¹; Haidy Metwally²; Robert G McAllister²; Vlad Popa²; ¹Univ. of Western Ontario, London, ON; ²Univ. of Western Ontario, London, Canada**
- WOB pm 03:10 **Multi-scale Simulations Coupled with Ion Mobility Experiments Reveal the Fate of nucleic Acids in the Gas Phase; Massimiliano Porrini^{1,2,3}; Clémence Rabin^{1,2,3}; Josephine Abi-Ghanem^{1,2,3}; Frédéric Rosu⁴; Valerie Gabelica^{1,2,3}; ¹INSERM-U1212, ARNA laboratory, Bordeaux, France; ²CNRS-UMR5320, ARNA laboratory, Bordeaux, France; ³Université de Bordeaux, IECB, ARNA laboratory, Pessac, France; ⁴CNRS UMS 3033, IECB, University of Bordeaux, Pessac, France**
- WOB pm 03:30 **How Important is the Charge Distribution in Ion Mobility Experiments, and Can We Predict It?; Jasper Boschmans¹; Filip Lemiere²; Frank Sobott³; ¹Owlstone, Cambridge, UK; ²University of Antwerp, Antwerp, Belgium; ³University of Antwerp, CGB V4, Antwerp, Belgium**
- WOB pm 03:50 **Polyproline Fragmentation in Negative Mode. What We Can Learn from Chemical Dynamics Simulations; Ana Martin-Somer¹; William L. Hase²; Riccardo Spezia³; ¹Université d'Evry-val-d'Essonne, Evry, France; ²Texas Tech University, Lubbock, TX; ³CNRS, Evry, Île-de-France**
- WOB pm 04:10 **Computations for the Gas-Phase Study of Macromolecular Structure; Erik G Marklund^{1,2}; Matteo T Degiacomi¹; Carol V Robinson¹; Michael Landreh¹; Mathieu Moog²; David Drew³; Carl Coleman^{2,4}; Andrew Baldwin¹; Justin L P Benesch¹; ¹University of Oxford, Oxford, UK; ²Uppsala University, Uppsala, SE; ³Stockholm University, Stockholm, Sweden; ⁴Center for Free-Electron Laser Science, Hamburg, Germany**

**2:30-4:30 pm WEDNESDAY
ENVIRONMENTAL: EMERGING CONTAMINANTS
Marc E. Engel (FDA, Food Safety Laboratories)
Stars Ballroom 1, level 3**

- WOC pm 02:30 **Hydraulic Fracturing Impacts on Drinking Water: High Resolution-MS Uncovers New Chemical By-Products; Susan Richardson¹; Hannah K. Liberatore²; Jeanne M. VanBriesen³; Plewa J. Michael⁴; Leslie H. Cizmas⁵; ¹University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; ²University of South Carolina, Columbia, SC; ³Carnegie Mellon University, Pittsburgh, PA; ⁴University of Illinois, Urbana, IL; ⁵Texas A&M, College Station, TX**
- WOC pm 02:50 **Heterogeneous Atmospheric Reactions: Identification of the Oxidation Products of Polycyclic Aromatic Hydrocarbons; Richard E. Cochran^{1,2}; Shokouh Haddadi^{1,3}; Rebeka Fisseha**

- Derseh¹; Alena Kubatova¹; ¹University of North Dakota, Grand Forks, ND; ²University of California San Diego, San Diego, CA; ³SUNY Oswego, Oswego, NY
- WOC pm 03:10 **Data-independent Mass Spectrometry for Development of Occupational Nanomaterial Exposure Biomarkers;** Andrew K. Ottens¹; Pretal P. Muldoon¹; Aleksandar Vucetic¹; Demetrius R. Carter¹; Stefan Tenzer²; Matthew J. Campen³; Aaron D. Erdely⁴; ¹Dept Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA; ²Institute of Immunology, University of Mainz, Mainz, Germany; ³Dept Pharmaceutical Sciences, University of New Mexico, Albuquerque, NM; ⁴National Institute for Occupational Safety and Health, Centers for Disease Control and Prevention, Morgantown, WV
- WOC pm 03:30 **Tracing Gadolinium-based Contrast Agents from Surface Water to Drinking Water by means of Speciation Analysis;** Uwe Karst¹; Marvin Birka²; Oliver Hachmöller²; Michael Sperling²; Christoph Alexander Wehe²; ¹University of Münster, Münster; ²University of Münster, Münster, DE
- WOC pm 03:50 **Determination of Unknown Dichlorophenols from the Oxidation of Triclosan Using Hydrogen Peroxide;** Matthew Reichert¹; Paul M Chiarelli¹; ¹Loyola University, Chicago, IL
- WOC pm 04:10 **Identification of Emerging Contaminants from a Waste Water Influenced Water Body Using High Resolution Accurate Mass LC/MS and Statistical Analysis;** Jerry Zweigenbaum¹; Tarun Anumol¹; Linda Kennedy²; ¹Agilent Technologies, Wilmington, DE; ²Mansfield University of Pennsylvania, Mansfield, PA

**2:30-4:30 pm WEDNESDAY
IMAGING: BIOMEDICAL APPLICATIONS
Bindesh Shrestha (Waters Corporation)
Stars Ballroom 2-3, level 3**

- WOD pm 02:30 **Guided DESI-MS Imaging Allows Accelerated Mapping of Heterogeneity in Breast Cancer;** Alessandra Tata¹; Michael Woolman¹; Milan Ganguly¹; Manuela Ventura¹; Nicholas Bernards¹; Adam Gribble²; Alex Vitkin²; Howard Ginsberg³; Arash Zarrine-Afsar²; ¹University of Health Network, Toronto, Canada; ²University of Toronto, Toronto ON, Canada; ³St. Michael Hospital, Toronto, Canada
- WOD pm 02:50 **Three-dimensional MALDI Imaging to Understand Metastasis in Pediatric Medulloblastomas;** Martin R L Paine¹; Jingbo Liu²; Danning Huang¹; Shane R Ellis³; Ron M A Heeren³; Facundo M Fernández¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Emory University School of Medicine, Atlanta, GA; ³Maastricht University, Maastricht, NL
- WOD pm 03:10 **Formalin-Fixed Paraffin Embedded Tissue Analysis by DESI-MSI and its Potential Use in Diagnostics;** Renata Soares¹; James McKenzie¹; Anna Mróz¹; Francesca Rosini¹; James L Alexander¹; Robert Goldin¹; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom
- WOD pm 03:30 **Redefining the Pathogen-host Interaction: Imaging Mass Spectrometry Reveals Staphylococcus Aureus Proteins within Host Tissues;** Jessica Moore¹; Neal D. Hammer²; Kristie M Lindsey Rose¹; Jeffrey M Spraggins¹; James Cassat³; Eric P Skaar³; Richard M Caprioli⁴; ^{1,5}; ¹Vanderbilt University MSRC, Nashville, TN; ²Michigan State University, East Lansing, MI;

- ³Vanderbilt University School of Medicine, Nashville, TN; ⁴Vanderbilt University, Nashville, TN; ⁵Vanderbilt Dept. of Biochemistry, Nashville, TN
- WOD pm 03:50 **Integrating Mass Spectrometry Imaging with Multiple Microscopy Modalities for Enhanced Spatiochemical Characterization of Dynamic Microbial Communities;** Sage J. B. Dunham¹; Kyungwon Ko¹; Nameera Baig²; Nydia Morales-Soto²; Troy J Comi¹; Bin Li¹; Joseph F Ellis¹; Joshua Shrout²; Paul W Bohn²; Jonathan V Sweedler¹; ¹University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ²University of Notre Dame, Notre Dame, IN
- WOD pm 04:10 **Biomedical Applications of Cardinal: a Mass Spectrometry Imaging Toolbox for Statistical Analysis;** April Harry¹; Kyle D Bemis¹; David Calligaris²; Nathalie Agar^{2,3}; Olga Vitek⁴; ¹Purdue University, West Lafayette, IN; ²Brigham and Women's Hospital, Boston, MA; ³Harvard Medical School, Boston, MA; ⁴Northeastern University, Boston, MA

**2:30-4:30 pm WEDNESDAY
TOP DOWN PROTEIN ANALYSIS
Si Wu (University of Oklahoma)
Stars Ballroom 4, level 3**

- WOE pm 02:30 **Comparing Electron Ionization Dissociation and Ultraviolet Photodissociation for Top-Down Native MS of Proteins and Protein Complexes;** Huilin Li¹; Yuewei Sheng¹; Jennifer S Brodbelt²; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA; ²University of Texas at Austin, Austin, TX
- WOE pm 02:50 **Elucidating Proteoform Families from Proteoform Intact Mass and Lysine Count Measurements;** Michael R. Shortreed¹; Brian L Frey¹; Mark Scalf¹; Rachel Knoener¹; Anthony J Cesnik¹; Lloyd M Smith¹; ¹University of Wisconsin Madison, Madison, WI
- WOE pm 03:10 **A Novel Approach to Sequencing Native Protein Complexes with an Orbitrap;** Mikhail Belov¹; ²; Philip D Compton³; Neil L Kelleher³; Stevan Horning⁴; Alexander A Makarov⁴; ¹Thermo Fisher Scientific (Bremen), Bremen, Germany; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Northwestern University, Evanston, IL; ⁴Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WOE pm 03:30 **Chemical Modification as a Path to Improved Top-down Sequencing and Structural Analysis of Proteins and Protein Complexes;** Daniel A. Polasky¹; Philip C Andrews²; ¹; Brandon T. Ruotolo¹; ¹Department of Chemistry, University of Michigan, Ann Arbor, MI; ²Department of Biological Chemistry, University of Michigan, Ann Arbor, MI
- WOE pm 03:50 **A Novel Top Down Proteomics Pipeline Utilizing Capillary Electrophoresis Separation and Ultraviolet Photodissociation;** Jolene K. Diedrich^{1,2}; Mathieu Lavallée-Adam¹; Qian Chu²; Bryan Fonslow³; ¹; James J Moresco^{1,2}; Alan Saghatelian²; John R Yates III^{1,2}; ¹The Scripps Research Institute, La Jolla, CA; ²The Salk Institute, La Jolla, CA; ³SCIEX, Brea, CA
- WOE pm 04:10 **Novel Strategies for Top-down Phosphoproteomics;** Bifan Chen¹; Leekyoung Hwang¹; Tania Guardado¹; William Ochowicz¹; Albert Chen¹; Cyrus Colah¹; Kunal Dani¹; Song Jin²; Ying Ge²; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin Madison, Madison, Wisconsin

2:30-4:30 pm WEDNESDAY
MS IN THE REGULATORY ENVIRONMENT
Jennifer Liu (Amgen)
Hemisfair Ballroom 3, level 3

- WOF pm 02:30 **The Use of Mass Spectrometry in FDA Applications for Biotherapeutics: A Retrospective Review;** Sarah Rogstad¹; Anneliese Faustino¹; David Keire²; Michael T Boyne³; Jun Park¹; ¹FDA, Silver Spring, MD; ²Food and Drug Administration, St. Louis, MO; ³Biotechlogie, Chicago, IL
- WOF pm 02:50 **The Roles and Opportunities for Mass Spectrometry in Regulatory CMC Submissions;** Heidi Zhang; Genentech, SSF, CA
- WOF pm 03:10 **Quantitative Analysis of Influenza Vaccine Antigens: How Does the Hi3 Method Compare to Methods Requiring Labeled Isotopes?**; Daryl G S Smith¹; Lisa Walrond¹; Marybeth Creskey¹; Genevieve Gingras¹; Yves Aubin¹; Caroline Gravel¹; Sean Li¹; Terry D Cyr¹; ¹Health Canada, Ottawa, Canada
- WOF pm 03:30 **Development of a LC-SRM Method Based on Anion Attachment Mass Spectrometry for Improved Detection of Neutral Anabolic Androgenic Steroids;** Quentin Dumont¹; Mariana Barcenat¹; Isabelle Bailloux²; Corinne Buisson²; Nathalie Mechin²; Richard B. Cole¹; ¹Sorbonne Universités, UPMC Univ Paris 06, Paris, France; ²Agence Française de Lutte Contre le Dopage, Châtenay-Malabry, France
- WOF pm 03:50 **NISTmAb Reference Material 8671: A Tool for Advancing Biopharmaceutical Mass Spectrometry;** John Schiel¹; Trina Formolo²; Abigail Turner²; Katharina Yandrowski²; ¹NIST, Gaithersburg, MD; ²NIST, Rockville, MD
- WOF pm 04:10 **The Challenges in Quantifying Tree Nut Residues of Phosphonic Acid and its Salts with LC-MSMS and CESI-MSMS;** Wiley Hall¹; Bill Beckham²; Spencer Walse³; Thomas Michael Jones²; Leonel Jimenez³; Alan Stone⁴; ¹DFA of California, Fresno, CA; ²DFA of California, Fresno, CA - California; ³USDA-ARS-CPQ, Parlier, CA - California; ⁴Johns Hopkins University, Baltimore, MD

2:30-4:30 pm WEDNESDAY
CARBOHYDRATES
John Froehlich (Boston Children's Hospital & Harvard Medical School)
Hemisfair Ballroom 2, level 3

- WOG pm 02:30 **Relative Quantification of Glycans using Multiplexed Carbonyl-Reactive Tandem Mass Tags and MultiNotch MS3;** Bingming Chen¹; Xuefei Zhong¹; Sergei Snovidat²; John Rogers²; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI; ²Thermo Fisher Scientific, Rockford, IL
- WOG pm 02:50 **Highly Sensitive N-and O-glycomics From Archived Formalin-Fixed Paraffin-Embedded (FFPE) Tissue Sections Using Porous Graphitized Carbon (PGC)-nanoLC-ESI-MS/MS;** Hannes Hinneburg^{1,2}; Petra Korac³; Slavko Gasparov^{4,5}; Peter H Seeberger^{1,2}; Vlatka Zoldos³; Daniel Kolarich¹; ¹Department of Biomolecular Systems, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany; ²Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Berlin, Germany; ³Faculty of Science, Department of Biology, Division of Molecular Biology, University of Zagreb, Zagreb, Croatia; ⁴Institute for Pathology and Cytology, University Hospital Merkur, Zagreb, Croatia; ⁵Department of Pathology, Medical

School Zagreb, University of Zagreb, Zagreb, Croatia

- WOG pm 03:10 **Measuring Variability of Glycosylation Analysis Methods for Monoclonal Antibodies: A NIST Interlaboratory Study;** M. Lorna A De Leoz¹; David Lee Duewer¹; Stephen E Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- WOG pm 03:30 **Strategies to Improve the Accuracy of De Novo Glycan Topology Analysis;** Cheng Lin¹; Pengyu Hong²; Yi Pu³; Catherine E. Costello^{1,3}; ¹Boston University School of Medicine, Boston, MA; ²Brandeis University, Waltham, MA; ³Boston University, Boston, MA
- WOG pm 03:50 **Oligosaccharide Isomer Discrimination by Ion Mobility Spectrometry and Tandem Mass Spectrometry: Roles of Metal Ion Adduction and Gas-Phase Ion Chemistry;** Eric D. Dodds¹; Yuting Huang¹; Katherine N. Schumacher¹; Abby S. Gelb¹; Lauren Petrosch¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WOG pm 04:10 **Temporal Glycan Analysis of IgG and Paraprotein from Multiple Myeloma Reveals Strong Pathological Associations with Altered Glycosylation;** Stefan Mittermayr¹; Gao Le^{1,2}; Peter O'Gorman³; Jonathan Bones¹; ¹The National Institute for Bioprocessing Research & Training, Dublin, Ireland; ²Department of Haematology, Mater Misericordiae University Hospital, Dublin, Ireland; ³Department of Haematology, Mater Misericordiae University Hospital, Dublin 7, Ireland, Dublin, Ireland

2:30-4:30 pm WEDNESDAY
NEW SEPARATIONS APPROACHES COUPLED TO MS
Michael L. Heien (University of Arizona)
Hemisfair Ballroom 1, level 3

- WOH pm 02:30 **Fundamentals of Ion Dynamics in Structures for Lossless Ion Manipulations (SLIM);** Sandilya V B Garimella¹; Yehia M Ibrahim¹; Ian K Webb¹; Ahmed M Hamid¹; Liulin Deng¹; Erin S Baker¹; Xueyun Zheng¹; Richard D Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA
- WOH pm 02:50 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry with the Third-Generation Electro-Kinetically Pumped Sheath Flow Interface for Large-Scale Proteomics;** Liangliang Sun¹; Katelyn R Ludwig²; Guijie Zhu²; Amanda B. Hummon²; Norman J Dovichi²; ¹University of Notre Dame, South Bend, IN; ²University of Notre Dame, Notre Dame, IN
- WOH pm 03:10 **A Novel Sensitive Sheathless CE-MS Device for Peptide and Protein Analysis;** Tam T. T. N. Nguyen¹; Nickolaj J. Petersen¹; Kasper D. Rand¹; ¹University of Copenhagen, Copenhagen, Denmark
- WOH pm 03:30 **Developing an Ultra UltraHigh Pressure Liquid Chromatography (UUHPLC) system for LC-MS Based Metabolomics;** Beixi Wang¹; Jeremy Felton¹; Paige Malec¹; Stephanie Moore²; James Treadway²; Dan Lunn²; James Jorgenson²; Robert Kennedy¹; ¹University of Michigan, Ann Arbor, MI; ²University of North Carolina at Chapel Hill, Chapel Hill, NC
- WOH pm 03:50 **Characterization of the Sarcomeric Proteome by Multidimensional Liquid Chromatography Fractionation and Top-down High-Resolution Mass Spectrometry;** Trisha Tucholski¹; Wenxuan Cai^{2,3}; Andrew J Alpert^{2,4}; Bifan Chen⁵; Yutong Jin⁵; Ying Ge^{2,5}; ¹Department of Chemistry, University of Wisconsin - Madison, Madison, WI; ²Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ³Molecular and

WOH pm 04:10

Cellular Pharmacology Training Program, University of Wisconsin - Madison, Madison, WI; ⁴PolyLC Inc., Columbia, MD; ⁵Department of Chemistry, University of Wisconsin-Madison, Madison, WI

Liquid Chromatography High Resolution Tandem Mass Spectrometry of Laser Ablation Sampled Tissue; Fabrizio Donnarumma¹; Michael E Pettit²; Touradj Solouki²; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA; ²Baylor University, Waco, TX

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

Jenny Brodbelt, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Stars Ballroom 1, level 3

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There are light refreshments in common areas.

01 Bioanalysis: Current Status of Strategy and Practice of a Tiered Approach (Regulated Bioanalysis Interest Group)
Fabio Garofolo and Jian Wang presiding
Room 220, level 2

The workshop will review the recent development and current status of strategy and practice of tiered approach in bioanalysis. The recommendations from various bioanalytical societies and organizations such as Global Bioanalytical Consortium (GBC) and European Bioanalytical Forum (EBF) and from Crystal City Conferences will be discussed. A pre-workshop survey will be conducted among ASMS members on the tiered approach in bioanalysis. The workshop will provide an opportunity for attendees to exchange opinions, experiences, and practices with the ultimate goal of having a better understanding of how to apply a tiered approach as part of the bioanalytical strategy.

02 Large-Scale Analysis of MS Big Data: From Data to Knowledge and Back
Nuno Bandeira presiding
Room 221, level 2

Advances in mass spectrometry instrumentation, integration with genomics/transcriptomics data and the public availability of hundreds of Terabytes of mass spectrometry data have created significant challenges for the analysis of proteomics and metabolomics data. This workshop will focus on publicly available algorithms and resources illustrating how distributed computing and mass spectrometry data repositories can be used to assist with the analysis of newly acquired data. Furthermore, we will also discuss ways to productively engage the mass spectrometry community in aggregating their contributions into a community-wide knowledge base reusable for both experimental design and continuous reanalysis towards complete annotation of public mass spectrometry data.

03 FTMS: Day-to-Day Concerns for High Resolution Mass Analysis (FTMS Interest Group)
David Kilgour and Don Smith presiding
Room 225A, level 2

This year's workshop will be a round-table discussion focusing on day-to-day considerations for optimum FTMS operation and data collection. A poll will be taken prior to the workshop to determine the most popular discussion points. In addition, there will be an open discussion on any other points of interest. What are the major opportunities to make the next generation of FTMS instruments better than the current ones? What are the most common day-to-day struggles that FTMS users encounter? Worried about mass calibration or mass errors? Bad or variable sensitivity? Instrument maintenance? Data processing and confidence in results? There are many more besides these. But, which are the most important to us as a community and can we use this information to shape our own future? Our aim will be to identify those key priority areas which might inform future programs for improving the capabilities offered by FTMS instrumentation.

04 Novel Mass Spectrometry Instrumentation: Moving into the Hands of Practitioners (Forensics & Homeland Security Interest Group)
Guido Verbeck presiding
Room 225B, level 2

Researchers are pushing the limits on trace forensic analysis and novel sampling techniques. They are also making mass spectrometry (MS) portable and durable for direct field applications; not just gas inlet, but liquid and solid sampling also. Recent developments in portable mass spectrometry present several interesting questions for workshop attendees to discuss. Questions for discussion include; Is it possible to create a reliable analytical tool that is "red light - green light"? Can portable MS become a tool that first responders can use without the need for extensive training? Will portable MS be considered a screening or a confirmatory method of analysis (e.g. by SWGDRUG) or will the error rates be measured (e.g. to meet Daubert requirements). How readily will portable MS be admissible in court? Could on-site measurements influence the way the criminal justice system operates and thereby save money?

Here we will explore these issues, and have a series of presentations that include portable MS developers and representatives from the practitioner/law enforcement perspectives. We will explore the courtroom, and what burden-of-proof is laid at the feet of the tool developer. A discussion will be moderated about moving portable MS forward as the presumptive test, as well as the prosecutorial final test.

05 Photoionization: New Developments (Photoionization MS Interest Group)
Jack Syage and Ralf Zimmermann presiding
Room 225C, level 2

This will be the fourth year for a Photoionization (PI) workshop. Previous ones were very successful with strong turnout and varied and vigorous discussions. There are two flavors of photoionization currently being practiced today: (1) atmospheric pressure photoionization (APPI) is a commercial technology and practiced mostly on LC/MS instrumentation though there are vibrant growing new applications in direct ambient analysis, GC/MS and direct vapor (or vaporized) sample analysis. (2) Vacuum photoionization more commonly referred to as single-photon ionization (SPI) involves VUV light sources including lasers that ionize sample inside the vacuum chamber and is more of a research tool for studying spectroscopic properties of molecules, but also finding powerful applications in air monitoring particularly pollutant monitoring such as vehicle or flue exhaust.

In this fourth year we will focus on new applications. APPI and PI are finding unique uses in high volume applications, most specifically explosives detection in security environments for its unique benefits that are not provided by competing ionization methods.

06 The NIH Review and Funding Process
Charles Edmonds, Salvatore Sechi, and
Douglas Sheeley presiding
Room 225D, level 2

A major source of financial support for many ASMS members and participants is the National Institutes of Health. During this workshop the general funding and review process of grant proposals will be presented. Issues like identifying the best NIH contact, writing an effective application, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH staff. Substantial time will be allotted for discussion and questions.

07 Entrepreneurship: Creating a Job in Mass Spectrometry
Alexandre Shvartsburg presiding
Room 301A, level 3

Much of the employment growth and technological advance in North America has lately come from start-ups. While spectacular successes of young companies in the IT and new media arena are widely covered and acclaimed, the entrepreneurial opportunities in other hi-tech areas are much less known. In mass spectrometry, start-ups have hugely contributed to the maturation of novel instrumentation and methods that define the frontline of our field and provided exciting and gainful employment for many analytical chemists including recent graduates.

This new ASMS workshop will focus on the key strategies and processes to create successful businesses leveraging the rapid development of MS technology and associated expansion of bioanalytical and environmental applications, and raise the awareness in broad ASMS community about entrepreneurship as a viable career path. The program would feature brief presentations by a diverse group of academic and industrial scientists who have launched prosperous ventures involving MS within the last two decades. Speakers will focus on key aspects of establishing a start-up in the field, such as funding, marketing, securing and protecting the intellectual property, licensing, staff hiring, manufacturing options, and relationships with major vendors. The workshop will conclude in a panel discussion with questions from the audience.

08 Protein Quantitation (Absolute) by LC-MS: Biomarker and Biotherapeutic
Dawn Dufield and Nalini Sadagopan presiding
Room 301BC, level 3

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.

09 Isomeric Glycans: Characterization & Quantitation
Yehia Mechref presiding
Room 302A, level 3

Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM). A correlation between changes in the glycan moieties of glycoproteins and many mammalian diseases, including hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been suggested. The diverse biological roles of glycans and their implications in diseases have created a demand for reliable glycomic strategies, permitting sensitive monitoring of isomeric glycans in biological systems. These strategies are needed to better understand the roles and attributes of glycan in biological systems. In

this workshop, the use of different MS/MS and LC-MS/MS strategies for the compressive characterization of glycan isomers will be critically described and discussed. These strategies employ several separation and mass spectrometric techniques, including liquid chromatography (different modes), matrix-assisted laser desorption ionization-mass spectrometry (MALDI-MS), and electrospray ionization-mass spectrometry (ESI-MS).

10 Protein Therapeutics: Characterization using MS
(Biotherapeutics Interest Group)
Damian Houde and Ashley Ruth presiding
Room 302BC, level 3

This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will begin with a discussion of hot topics identified at this year's Sanibel Conference on Protein Therapeutic Characterization. This may include a variety of topics, ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.

11 The Exposome: MS-based Metabolomic Workflows to Characterize the Exposome (Exposomics Interest Group)
Anthony Macherone presiding
Room 303A, level 3

The exposome complements the genome and integrates genetic information with non-genetic exposures and the associated biological response pathways in the search for causative factors of chronic human disease. Within the exposome paradigm, the internal environment is composed of all bio-active chemicals circulating in the body regardless of their origin e.g. genetically derived or exposure derived. Examples include dietary chemicals, drugs, persistent organic pollutants, bio-transformation products (metabolites), foreign DNA, reactive electrophiles adducted to human serum albumin and other sources of exposure (e.g., noise pollution, place of residence, lifestyle choices, etc.) that stimulate biochemical responses.

Exposomics is the application of omics-based tools such as NMR, mass spectrometry and bioinformatics to characterize and measure the exposome and applies the tools of systems biology in a truly multi-platform, multi-omics approach. Mass spectrometric workflows in metabolomics and the bioinformatics software required to interpret the resulting data, provide an excellent model for the characterization of the exposome. This workshop will define how metabolomic procedures and workflows can be used to characterize human exposure profiles and will provide examples used to characterize the exposome.

12 Biomarker Translation: Quality Control & Quality Assurance (Clinical Chemistry Interest Group)
Timothy Garrett and Brian Rappold presiding
Room 303BC, level 3

Quality control and quality assurance (QC/QA) procedures for translating discovery assays to clinical use are poorly, if at all, defined. This workshop will offer brief topic introductions regarding the expectations of QC/QA in clinical diagnostics for multimarker assays, including algorithm based assessments. A similar dearth of QC/QA procedures is found in technologies which are highly naive to the industry, such as high resolution MS and tissue/imaging. As such, speakers from the field will introduce concepts related to QC/QA in such methodologies to enable discussion amongst the group. Hopefully, such discussion will introduce new approaches to ensuring quality in translational workflows for all attendees.



13 Imaging MS: Present and Future of Multimodal Studies
(Imaging MS Interest Group)
Vilmos Kertesz and Raf Van de Plas presiding
Room 304, level 3

It is increasingly common for Imaging MS to make up part of multimodal imaging studies in which a set of different image types are brought to bear on the same or related samples. Analytical approaches that characterize a sample using different principles, measuring for example functional, chemical, as well as biological information within a single experiment, can often provide insights not available from a single modality alone. While multimodal imaging that includes a mass spectral modality has greatly advanced, different research groups have gone about such studies with widely-varying workflows and approaches. In this workshop, we want to discuss how challenges can be tackled at the sample preparation, at the instrumental, as well as at the computational level. Furthermore, we want to see whether an overall direction for the field and a set of best practices can be distilled, complemented by a list of major challenges that yet need to be tackled. The central topic of the workshop will therefore be "Imaging by Mass Spectrometry as part of Multimodal Imaging Studies".

The workshop proposes to examine three different aspects of multimodal imaging MS experiments:

1. Experimental design - How to design a good multimodal imaging MS experiment? (e.g. What modalities to acquire? How to make the collected image types synergistic and not just a simple combination?)
2. Measurement - How to acquire the different image types? (e.g. How do you properly prepare the sample for multimodal measurements? Is it better to integrate mass spectrometry and other image type measurements into a single device? Or are we better off keeping separate instruments?)
3. Data analysis - How can multimodal data be brought together, and what are the advantages and disadvantages of the different approaches? (e.g. What are the different strategies to handle/visualize multimodal data sets?)

14 Galaxy for Proteomics Data Analysis:
An Interactive Demonstration
Tim Griffin presiding
Room 305, level 3

The Galaxy framework has emerged as a useful and powerful tool for MS-based proteomics data analysis and also multi-omic application (for example see recent publications such as Nat Biotechnol. 2015, 33:137-9; Mol Cell Proteomics. 2015, 14:3087-93; Mol Cell Proteomics. 2012, 11:M111.015974). The Galaxy operating environment offers an informatics workbench where disparate software can be deployed and integrated into complex workflows. Galaxy also offers the ability to share complete workflows and data with other users, promoting reproducibility and dissemination of even complex data analysis schemes.

This workshop will provide attendees the opportunity to take Galaxy for a "test drive" in analyzing MS-based proteomics data. Attendees will have the opportunity to access a Galaxy instance and walk through the basic steps of setting up an analysis of representative MS data from a proteomics experiment. The hands-on tutorial will include steps such as pre-processing of mass spectral data, sequence database searching, and filtering and visualizing outputs.

Attendees will also be introduced to basic operations and concepts of the Galaxy operating environment, such as the creation of histories and workflows, and functionalities for sharing tools and workflows with others. An overview of the current state of software available in Galaxy for proteomics and multi-omics applications will also be provided.

The workshop will be led by both developers and users well-versed in the use of Galaxy for multi-omics data analysis.

Attendees are encouraged to bring a laptop computer to participate.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
GRAND HYATT HOTEL

THURSDAY MORNING ORAL SESSIONS

8:30-10:30 am THURSDAY
NEW CONCEPTS FOR FORENSIC MS
Candice Bridge (National Center for Forensic Science)
Hall 1, level 1

- ThOA am 08:30 **Paper Spray Mass Spectrometry for Screening of Illicit Drugs from Blood Samples;** Rachel Potter¹; Nicholas Manicke¹; ¹IUPUI, Indianapolis, IN
- ThOA am 08:50 **Comparative Study for the Authentication of Marijuana Varieties by Conventional and High-Resolution Mass Spectrometric Profiling;** Xinyi Wang¹; Peter B Harrington¹; Steven F Baugh²; ¹Ohio University, Athens, OH; ²Cannaprint, LLC, Broomfield, CO
- ThOA am 09:10 **Coupling Ambient Ionization and In-source Collision Induced Dissociation for the Detection and Chemical Imaging of Organic and Inorganic Forensic Compounds;** Thomas P. Forbes¹; Edward Sisco¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- ThOA am 09:30 **Classification of Blow Fly Eggs for Determination of Post-Mortem Interval;** Justine E. Giffen¹; Jennifer Y. Rosati²; Rabi A. Musah³; ¹University at Albany - SUNY, Albany, NY; ²John Jay College of Criminal Justice, NY, NY; ³University at Albany-SUNY, Albany, NY
- ThOA am 09:50 **Proteomics and Ancient History - Identification of Proteins from Skin and Muscle Tissue from Ancient Egyptian Mummies;** Prathiba

Ravishankar¹; Dylan Xavier²; Fallen Kai Yik Teoh¹; David C.L. Handler¹; Mads Moeller Foged¹; Mehdi Mirzaei¹; Dong Hoon Shin³; Raffaella Bianucci⁴; Jana Jones¹; Paul A Haynes⁵; ¹Macquarie University, Sydney, Australia; ²Australian Proteome Analysis Facility, Sydney, Australia; ³Seoul National University, Seoul, South Korea; ⁴University of Turin, Torino, Italy; ⁵Macquarie University, North Ryde, Sydney, NSW

- ThOA am 10:10 **Illuminating Lifestyles of People by Metabolomics of Personal Objects;** Amina Bouslimani¹; Alexey V Melnik¹; Zhenjiang Zech Xu¹; Amnon Amir¹; Ricardo Silva^{1,2}; Mingxun Wang¹; Nuno Bandeira¹; Theodore Alexandrov^{3,4}; Rob Knight¹; Pieter Dorrestein¹; ¹UCSD, San Diego, CA; ²Universidade de São Paulo - USP, São Paulo, Brazil; ³EMBL Heidelberg, Heidelberg, Germany; ⁴SCiLS GmbH, Bremen, Germany

8:30-10:30 am THURSDAY
FUNDAMENTALS: PHOTODISSOCIATION
John P. O'Brien (The Dow Chemical Company)
Room 221, level 2

- ThOB am 08:30 **Diazirine Enabled Gas Phase Coupling of Peptides Utilizing Newly Developed Photo-Lysine Amino Acid;** Robert Pepin¹; Christopher L Shaffer¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA

- ThOB am 08:50 **Conformational Specific Infrared and Ultraviolet Spectroscopy of Cold YA(D-Pro)AA-H+Ions: A Stereochemical "Twist" on the Proline Effect;** Christopher Harrihal¹; Andrew DeBlase¹; Nicole Burke¹; Timothy Zwier¹; Scott A McLuckey¹; ¹*Purdue University-Department of Chemistry, West Lafayette, IN*
- ThOB am 09:10 **Examination of the Asymmetric and Symmetric Dissociation Pathways of Tetrameric Protein Complexes using 193 nm UVPD;** Lindsay Morrison¹; Jennifer S Brodbelt¹; ¹*University of Texas at Austin, Austin, TX*
- ThOB am 09:30 **UVPD on the Benchtop Q Exactive Orbitrap Applied to Peptides, Proteins, and Protein Complexes;** Kyle Fort¹; Sam Tamara¹; Andrey Dyachenko¹; Alexander A Makarov^{2,1}; Richard Scheltema¹; Albert J R Heck¹; ¹*Utrecht University, Utrecht, The Netherlands*; ²*Thermo Fisher Scientific, Bremen, DE*
- ThOB am 09:50 **From the Top to the Bottom and Back: hvPD on Conformer Selected Ions Probing the Role of Co-factors of Structure;** Alina Theisen¹; Bin Yan¹; Rodger Kutta¹; Alex Jones¹; Bruno Bellina¹; Perdita E Barran²; ¹*The University of Manchester, Manchester, United Kingdom*; ²*The University of Manchester, Manchester, Greater Manchester*
- ThOB am 10:10 **Performance Considerations for Ultraviolet Photo-Dissociation using the Nd:YAG 5th Harmonic (213nm);** Chad Weisbrod¹; Eugene Zhuk¹; Jean-Jacques Dunyach¹; Jae Schwartz¹; ¹*ThermoFisher Scientific, San Jose, CA*
- 8:30-10:30 am THURSDAY
NEW DEVELOPMENTS IN IONIZATION AND
SAMPLING FOR DMPK
Naidong Weng (Johnson & Johnson)
Stars Ballroom 1, level 3**
- ThOC am 08:30 **Coated Blade Spray-Mass Spectrometry (CBS-MS) as a Versatile Approach for Quantitative Analysis in Small and Large Sample Volumes of Biofluids;** German Augusto Gomez-Rios¹; Nathaly Reyes-Garcés¹; Ezel Boyacı¹; Justen Poole¹; Janusz Pawliszyn¹; ¹*University of Waterloo, Waterloo ON, Canada*
- ThOC am 08:50 **Functionalized Sampling Probe for Direct Mass Spectrometry Analysis of Lipids in Blood Samples;** Wenpeng Zhang¹; Zheng Ouyang¹; ¹*Biomedical Engineering, Purdue University West Lafayette, IN*
- ThOC am 09:10 **Microfluidic Electrochemical Cell for Studying the Adduct Formation of Reactive Metabolites by ESI-MS;** Tina Wigger^{1,2}; Floris T.G. van den Brink³; Mathieu Odijk³; Wouter Olthuis³; Albert van den Berg³; Uwe Karst^{1,2}; ¹*University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany*; ²*NRW Graduate School of Chemistry, Münster, Germany*; ³*University of Twente, MESA+ Institute for Nanotechnology and MIRA Institute for Biomedical Technology and Technical Medicine, BIOS – Lab on a Chip group, Enschede, The Netherlands*
- ThOC am 09:30 **Effective Coupling of CE with nanoESI MS via a True Sheathless Metal-coated Emitter Interface for Robust and Sensitive Sample Quantification;** Keqi Tang¹; Xuejiang Guo²; Thomas Fillmore¹; Yuqian Gao¹; ¹*Pacific NW National Laboratory, Richland, WA*; ²*Nanjing University, Nanjing, China*
- ThOC am 09:50 **Novel Acoustic Interface for Ultra-High-Throughput Mass Spectrometry Utilizing Multiple Ambient Ionization Techniques;** Ian Sinclair¹; Jonathan Wingfield²; Martin Bachman¹; Steven D Pringle³; Luke Ghislain⁴; Eric Hall⁴; Rick Stearns⁴; Sammy Datwani⁴; Lars Majlof⁴; Michael Morris³; ¹*AstraZeneca, Macclesfield, UK*; ²*AstraZeneca, Cambridge, UK*; ³*Waters, Wilmslow, United Kingdom*; ⁴*Labcyte Inc, Sunnyvale, CA - California*
- ThOC am 10:10 **Sub Second Quantitative Mass Spectrometry Analysis No Longer a Fiction with Acoustic Sample Deposition and Fiber Coupled LDTD-MS/MS;** Pierre Picard¹; Jean Lacoursière¹; Alex Birsan¹; Serge Auger¹; ¹*Phytronix Technologies, Inc. Quebec, Canada*
- 8:30-10:30 am THURSDAY
TRANSLATIONAL SUCCESS WITH MS
Ashok R. Dongre (Bristol-Myers Squibb R&D)
Stars Ballroom 2-3, level 3**
- ThOD am 08:30 **Pathology-driven Comprehensive Proteomic Profiling of the Prostate Cancer Tumor Microenvironment;** Lisa Staunton¹; Claire Tonry¹; Espina Virginia²; Lance Liotta²; John O'Leary³; Rosina Lis⁴; Michaela Bowden⁴; Finn Stephen³; Massimo Loda⁴; Stephen Pennington⁵; ¹*University College Dublin, Dublin, Ireland*; ²*George Mason University, Manassas, Virginia*; ³*Trinity College Dublin, Dublin, Ireland*; ⁴*Dana Farber Cancer Institute, Boston, MA*; ⁵*UCD Conway Institute, Dublin, Europe*
- ThOD am 08:50 **Development of a Novel Rapid Evaporative Ionisation Mass Spectrometry (REIMS) Platform 'iEndoscope' for in vivo Chemical Histology during Colonoscopy;** James Alexander¹; Louise Gildea¹; Julia Balog²; Abigail Speller¹; Anna Mroz¹; Alasdair Scott¹; James McKenzie¹; Kirill Veselkov¹; Robert Goldin¹; James Kinross¹; Jonathan Hoare¹; Julian P Teare¹; Zoltan Takats¹; ¹*Imperial College, London, United Kingdom*; ²*Waters, Manchester, United Kingdom*
- ThOD am 09:10 **Rapid Identification of Carbapenem-resistant Klebsiella Pneumoniae using High-Resolution Tandem Mass Spectrometry;** Raja Sekhar Nirujogi¹; Sreelakshmi K Sreenivasamurthy¹; Santosh Renuse¹; Pranita J Tamma¹; Patricia J Simner¹; Akhilesh Pandey¹; ¹*Johns Hopkins University School of Medicine, Baltimore, MD*
- ThOD am 09:30 **Ultrafast Detection of Amino-Acid Substitutions in DNA Gyrase A Related to Fluoroquinolone Resistant Typhoidal Salmonella Isolates using PRM;** Robert-Jan Hassing¹; Wil Goessens¹; Lona Zeneyedpour¹; Sadaf Sultan¹; Jeroen van Kampen¹; Annelies Verbon¹; Perry van Genderen²; John Hayes¹; Theo Luider¹; Lennard Dekker¹; ¹*Erasmus Medical Center, Rotterdam, The Netherlands*; ²*Havenziekenhuis, Rotterdam, The Netherlands*
- ThOD am 09:50 **A Physical and Genetic Interaction between the Cardiac Transcription Factor Tbx5 and Chromatin Remodeling Complexes is Essential for Cardiac Septation;** Todd M. Greco¹; Lauren Waldron²; Jeffrey D. Steimle³; Nicholas C. Gomez⁴; Kerry M. Dorr²; Junghun Kweon³; Brenda Temple⁵; Xinan Holly Yang³; Caralynn M. Wilczewski²; Ian J. Davis⁶; Ivan P. Moskowitz³; Frank L. Conlon²; Ileana M. Cristea¹; ¹*Princeton University, Princeton,*

NJ; ²University of North Carolina Heart Institute, UNC-Chapel Hill, Chapel Hill, NC; ³Departments of Pediatrics, Pathology, and Human Genetics, The University of Chicago, Chicago, IL; ⁴Integrative Program for Biological and Genome Science, UNC-Chapel Hill, Chapel Hill, NC; ⁵R.L. Juliano Structural Bioinformatics Core, Department of Biochemistry and Biophysics, UNC-Chapel Hill, Chapel Hill, NC; ⁶Department of Genetics, UNC-Chapel Hill, Chapel Hill, NC

ThOD am 10:10 **Discovery and Mechanistic Investigation of Novel Metabolic Features of Lung Cancer and Their Potentials of Clinical Applications;** Hyuntae Yoo¹; Tzu-Fang Lou¹; Deepa Sethuraman¹; Pallevi Srivastva¹; John Minna²; ¹University of Texas at Dallas, Richardson, TX; ²University of Texas Southwestern Medical Center, Dallas, Texas

**8:30-10:30 am THURSDAY
GLYCOPEPTIDES AND GLYCOPROTEINS
Franklin E. Leach III (Photochem Technologies)
Stars Ballroom 4, level 3**

ThOE am 08:30 **Dopant Enriched Nitrogen Gas Enhances Sensitivity and Repeatability, Opening New Possibilities for Glyco(proteo)mics Analysis with Sheathless CE-ESI-MS;** Guinevere S.M. Kammeijer¹; Isabelle Kohler¹; Bas C. Jansen¹; Gerda C.M. Vreeker¹; Paul J. Hensbergen¹; Oleg A. Mayboroda¹; David Falck¹; Manfred Wuhrer¹; ¹Leiden University Medical Center (LUMC), Leiden, Zuid-Holland

ThOE am 08:50 **Comprehensive Glycoproteomics of Glioblastoma Biospecimens;** Chun Shao¹; Joshua Klein¹; Joanna Phillips²; Joseph Zaia¹; ¹Department of Biochemistry, School of Medicine, Boston University, Boston, MA; ²Department of Neurological Surgery and Pathology, University of California, San Francisco, San Francisco, CA

ThOE am 09:10 **Quantification of Human Cell Surface N-Glycoprotein Dynamics;** Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, USA

ThOE am 09:30 **Isomeric Separation of Glycopeptides using Aporous Graphitic Carbon (PGC) LC-MS Platform;** Rui Zhu¹; Jingfu Zhao¹; Aiyang Yu¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas

ThOE am 09:50 **Site-directed Analysis of Unnatural Glycopeptide Variants and the Associated Glycan Structures by Semi-Targeted LC/MS and MRM Analysis;** Dayoung Park¹; Gege Xu¹; Carlito B Lebrilla¹; ¹UC Davis, Davis, CA - California

ThOE am 10:10 **Quantitative Profiling of O-GlcNAc Glycosites in Human T Cells during Activation;** Christina Woo¹; Peder J Lund²; Sharon J Pitteri²; Mark M Davis^{2,3}; Carolyn R Bertozzi^{1,3}; ¹Stanford University, Stanford, CA; ²Stanford University School of Medicine, Palo Alto CA, USA; ³Howard Hughes Medical Institute, Chevy Chase, MD

**8:30-10:30 am THURSDAY
INFORMATICS: TARGETED PROTEOMICS AND DIA
Hannes L. Röst (IMSB, ETH Zurich & Stanford University)
Hemisfair Ballroom 3, level 3**

ThOF am 08:30 **EncyclopeDIA: a New Algorithmic Approach to Detect, Site-Localize, And Quantify Phosphopeptide Positional Isomers from DIA Experiments;** Brian C. Searle^{1,2}; Robert T Lawrence¹; Michael J MacCoss¹; Judit Villén¹; ¹University of Washington, Seattle, WA; ²Proteome Software, Portland, OR

ThOF am 08:50 **A Novel Framework for Spectral Assay Library Construction and Targeted Quantitative Data Extraction in Metabolomics with Data Independent Acquisition;** Gengbo Chen¹; Scott Walmsley²; Lei Zhou^{1,3,4}; Liyan Chen³; Ching-Yu Cheng^{3,4}; Roger W Beuerman^{3,4}; Tien-Yin Wong^{1,3,4}; Gemmy C.M. Cheung^{3,4}; Hyungwon Choi¹; ¹National University of Singapore, Singapore, Singapore; ²University of Colorado Denver-Anschutz In Aurora, CO, Denver, USA; ³Singapore Eye Research Institute, Singapore, Singapore; ⁴Duke-NUS Graduate Medical School, Singapore, Singapore

ThOF am 09:10 **Targeted Analysis of MS1 Data for Quantitative Studies;** Roland M. Bruderer¹; Yue Xuan²; Ian Lienert¹; Oliver M. Bernhardt¹; Tejas Gandhi¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland; ²Thermo Fisher Scientific, Bremen, DE

ThOF am 09:30 **Benchmarking SWATH by LFQ-Bench: a Multi-Centered Study Evaluates and Improves Data-Independent-Acquisition-Based Label Free Quantification Tools;** Pedro Navarro¹; Joerg Kuharev¹; Ludovic C Gillet²; Oliver M Bernhardt³; Brendan MacLean⁴; Stephen Tate⁵; Chih-Chiang Tsou⁶; Lukas Reiter³; George Rosenberger²; Yasset Perez-Riverol⁷; Alexey I Nesvizhskii⁶; Ruedi Aebersold²; Stefan Tenzer¹; ¹University Medical Center of the Johannes Gutenberg, Mainz, Rheinland-Pfalz; ²ETH Zurich, Zurich, Switzerland; ³Biognosys AG, Schlieren, Switzerland; ⁴University of Washington, Seattle, WA; ⁵SCIEX, Concord, ON; ⁶University of Michigan, Ann Arbor, MI; ⁷EMBL-EBI, Hinxton, UK

ThOF am 09:50 **Advanced Workflows and Concepts for the Analysis of High Throughput Targeted Proteomics Experiments of Large Heterogeneous Datasets;** Isabell Bludau¹; George Rosenberger¹; Ben Collins¹; Uwe Schmidt²; Patrick Pedrioli¹; Ruedi Aebersold¹; ¹Institute of Molecular Systems Biology, ETH Zurich, Zurich, CH; ²ID Scientific IT Services, ETH Zurich, Zurich, CH

ThOF am 10:10 **Detection and Quantification of Proteins in SWATH-MS Analysis without using Spectral Libraries;** Stephen A Tate¹; Jamie Sherman¹; Pradeep Narayanaswamy¹; ¹SCIEX, Concord ON, Canada

**8:30-10:30 am THURSDAY
APPLICATION OF STABLE ISOTOPE LABELING IN MS
Jim Edwards (Saint Louis University)
Hemisfair Ballroom 2, level 3**

ThOG am 08:30 **Quantity: An Isobaric Tag for Quantitative Glycomics;** Shuwei Li¹; Shuang Yang²; Meiyao Wang³; Lijun Chen²; Bojiao Yin²; Karen W Phinney⁴; Illarion V Turko⁴; Michael Betenbaugh²; Guoqiang Song⁵; Chung Cheng-yu⁶; Hui Zhang²; ¹Center for Advanced Research, Rockville, MD; ²Johns Hopkins School of Medicine, Baltimore, MD; ³Center for Disease Control and Prevention, Atlanta, GA; ⁴National Institute of Standards and Technology, Gaithersburg, MD; ⁵Changzhou University, Changzhou, China; ⁶Johns Hopkins University School of Medicine, Baltimore, MD

ThOG am 08:50 **A Novel Quantitative Mass Spectrometry Platform for Determining Protein O-GlcNAcylation Dynamics through Specific O-GlcNAc Isotopic Labeling;** Xiaoshi Wang¹; Zuo-Fei Yuan¹; Jing Fan²; Kelly R Karch¹; Lauren E Ball³; John M Denu²; Benjamin A Garcia⁴; ¹University of Pennsylvania School Of Medicine, Philadelphia, PA; ²University of Wisconsin Madison, Madison,

Wisconsin; ³Medical Univ of S Carolina, Charleston, SC; ⁴University of Pennsylvania School of Medicine, Philadelphia, PA

- ThOG am 09:10 **High-Performance Chemical Isotope Labeling LC-MS for Tracking Disease Progression: Metabolomic Study of Alzheimer's Disease in a Mouse Model;** Liang Li¹; Wei Han¹; Kevin Hooton¹; Dorothea Mung¹; Keding Cheng²; Sharon Simon²; David Knox²; ¹University of Alberta, Edmonton, Canada; ²Public Health Agency of Canada, Winnipeg, Canada
- ThOG am 09:30 **An Integrated Workflow for Qualitative Flux Analysis by Accurate Mass LC/MS;** Stephen Madden¹; Alex Appfel¹; Xinning Jiang²; Ed Darland²; Yinghang Yang²; Xiangdong Li²; Crystal Cody²; Norton Kitagawa²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Santa Clara, CA
- ThOG am 09:50 **HAHA: A Novel Strategy for Quantification of Newly Synthesized Proteins;** Yuanhui Ma¹; Daniel B Mcclatchy¹; John Yates¹; ¹The Scripps Research Institute, La Jolla, CA
- ThOG am 10:10 **Just Add Water and Resolving Power: Metabolic Labeling and MS Techniques for Lipid and Intact Protein Quantitation in Any Organism;** Nicholas D Schmitt¹; Jeniffer Quijada¹; Christopher Thompson²; Michael L Easterling²; Jeffrey Agar¹; ¹Northeastern University, Boston, MA; ²Bruker Daltonic, Billerica, MA

**8:30-10:30 am THURSDAY
ION MOBILITY: STRUCTURE**
Kevin Pagel (Freie Universitaet Berlin)
Hemisfair Ballroom 1, level 3

- ThOH am 08:30 **An Ion Mobility, Molecular Dynamics, Top-Down and H/DX Study of Monoclonal Antibody Structural Collapse in the Gas-phase;** Iain D G Campuzano¹; Morgan Lawrenz¹; Carlos Larriba-Andaluz²; Huilin Li³; Ulrik H Mistar⁴; Kasper Rand⁴; Joseph Loo³; ¹Amgen, Inc., Thousand Oaks, CA; ²Indiana University-Purdue University, Indianapolis, IN; ³UCLA, Los Angeles, CA; ⁴University of Copenhagen, Copenhagen, Denmark
- ThOH am 08:50 **Analysis of Protein Structural Changes with High Resolution Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-Mass Spectrometry;** Ian K. Webb¹; Liulin Deng²; Ahmed M Hamid¹; Gordon A Anderson^{1,3}; Randolph V Norheim¹; Spencer A Prost¹; Sandilya V. B. Garimella¹; Erin S Baker¹; Yehia M Ibrahim¹; Richard D Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, wa; ³GAA Custom Engineering, Benton City, WA
- ThOH am 09:10 **Ubiquitin Ion Structures from the Solid State using Nothing More than a Small Molecule and Vacuum of an IMS-MS Instrument;** Ellen D. Inutan^{1,2}; Tarick J. El-Baba³; Casey D. Foley²; David E. Clemmer³; Sarah Trimpin^{2,4}; ¹Mindanao State University-Iligan Institute of the Technology, Iligan City, Philippines; ²Department of Chemistry, Wayne State University, Detroit, MI; ³Department of Chemistry, Indiana University, Bloomington, IN; ⁴Cardiovascular Research Institute, Wayne State University School of Medicine, Detroit, MI
- ThOH am 09:30 **Combining Ion Mobility with Cryogenic Ion Spectroscopy for Studying Peptide Structure on the Way from Solution to the Gas Phase;** Liudmila Voronina¹; Antoine Masson²; Michael Kamrath¹; David E Clemmer³; Carsten Baldauf⁴; Thomas R Rizzo¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ²UC Berkeley, Berkeley,

California; ³Indiana University Dept. Chemistry, Bloomington, IN; ⁴Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

ThOH am 09:50 **Insights from TIMS-MS, IR Spectroscopy and Molecular Dynamics on Nicotinamide Adenine Dinucleotide Structural Dynamics: NAD+vs NADH;** Juan Camilo Molano¹; Walter Gonzalez¹; Jaroslava Miksovska¹; Philippe Maitre²; Francisco Fernandez Lima¹; ¹Florida International University, Miami, FL; ²Laboratoire de Chimie Physique, Orsay, Orsay, France

- ThOH am 10:10 **Polymers as Model Systems to Understand Ion Mobility Mass Spectrometry Structures in Gas Phase;** Jean R. N. Haler¹; Denis Morsa¹; Johann Far¹; Christine Jérôme²; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; ²CERM, University of Liege, Liege, Belgium

**10:30 AM – 2:30 PM, THURSDAY
THURSDAY POSTER SESSION**
Poster/Exhibit Hall

Lunch concessions are open 11:00 am – 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

THURSDAY AFTERNOON ORAL SESSIONS

**2:30-4:30 pm THURSDAY
FOOD SAFETY AND CHEMISTRY: NON-TARGETED
SCREENING**

Juan F. García-Reyes (University of Jaen)
Hall 1, level 1

- ThOA pm 02:30 **Comprehensive Pesticide Screening in Complex Matrices by Collision Cross Section using a Novel Geometry Travelling-Wave IMS-QToF Mass Spectrometer;** Olivier Saperas¹; Brigitte Ogundejai¹; Jennifer Unsworth²; Nick Tomczyk²; Martin Palmer²; Darren Hewitt²; Christophe Siroit²; Davy Petit²; Daniel J. Weston²; ¹Lacapa, Toulouges, France; ²Waters, Wilmslow, United Kingdom
- ThOA pm 02:50 **Main Challenges in LC-HRAMS Method Development for Pesticide Residue Analysis;** Łukasz Rajski¹; María del Mar Gómez Ramos¹; Amadeo R Fernández-Alba¹; Maciej P Bromirski²; ¹European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables. University of Almeria, Agrifood Campus of International Excellence (ceiA3), Almeria, Spain; ²Thermo Fisher Scientific, San Jose CA, CA - California
- ThOA pm 03:10 **Characterization of Iodine Containing Disinfection By-Products in Water using Gas Chromatography Orbitrap-based Mass Spectrometry;** Cristina Postigo¹; Cristian Cojocariu²; Susan D Richardson³; Damia Barcelo⁴; Paul Silcock²; ¹Institute for Environmental Assessment and Water Research - Spanish National Research Council (IDAEA-CSIC), Barcelona, Spain; ²Thermo Fisher Scientific, Runcorn, UK; ³University of South Carolina, Columbia, SC; ⁴ICRA, Girona, Spain
- ThOA pm 03:30 **GC x GC x Q-TOF-MS Survey of Essential Oils;** Edward Ledford¹; Zhanpin Wu²; Sofia Nieto³; Stephen E Reichenbach⁴; Qingping Tao⁵; ¹Zoex Corporation, Houston, TX; ²Zoex Corporation, Lincoln, NE; ³Agilent Technologies, Santa Clara, CA; ⁴Dep. of Computer Science and Engineering, University of Nebraska at Lincoln, Lincoln, NE; ⁵GC Image, LLC Lincoln, NE



THURSDAY AFTERNOON ORAL SESSIONS

ThOA pm 03:50 **Instantaneous Determination of Cocoa Content and Cocoa Bean origin of Commercial Products with Rapid Evaporative Ionization Mass Spectrometry**; Julia Balog^{1,2}; Richard Schäffer¹; Tamas Juhasz¹; Tamas Karancsi¹; Steven D Pringle³; Zoltan Takats²; ¹Waters Research Centre, Budapest, Hungary; ²Imperial College London, London, United Kingdom; ³Waters, Wilmslow, United Kingdom

ThOA pm 04:10 **Classification of Olive Oils using Direct Analysis Atmospheric Pressure Chemical Ionization-Mass Spectrometry**; Pilar Perez-Hurtado¹; Amy Giles¹; Mark Allen²; Lourdes Arce³; Matthew Turner¹; Jim Reynolds⁴; ¹Loughborough University, Loughborough, United Kingdom; ²Advion UK Ltd, Essex, United Kingdom; ³Universidad de Cordoba, Cordoba, SPAIN; ⁴Loughborough University, Loughborough, Leicestershire

2:30-4:30 pm THURSDAY

FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION

Arpad Somogyi (The Ohio State University)

Room 221, level 2

ThOB pm 02:30 **Charge Transfer Dissociation (CTD): High Energy Radical Fragmentation of Glycans, Peptides and Lipids**; Glen Paul Jackson¹; Iris Kreft¹; Pengfei Li¹; David Ropartz²; Hélène Rogniaux²; ¹West Virginia University, Morgantown, WV; ²INRA, UR1268 Biopolymers Interactions Assemblies Nantes, France

ThOB pm 02:50 **Improvement of Hydrogen Attachment/ Abstraction Dissociation (HAD) Efficiency for Low-Charged Peptides using Supplemental Activation**; Hidekazu Takahashi¹; Sadanori Sekiya¹; Takashi Nishikaze¹; Shosei Yamauchi¹; Shinichi Iwamoto¹; Motoi Wada²; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Doshisha University, Kyotanabe, Japan

ThOB pm 03:10 **Conformational Effects on the Dissociation Kinetics of Proton-Bound Heterodimer Ions: Applications to Gas-Phase Acidities of Alkanols**; Kent M. Ervin¹; Jerry G Lanorio¹; Surja B Ghale²; Alex A Nickel²; ¹University of Nevada, Reno, Reno, NV; ²University of Nevada, Reno, Reno, NV

ThOB pm 03:30 **Mobile C-H Protons in a Proton Deficient Peptide**; Damodar Koirala¹; Paul G Wenthold²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN

ThOB pm 03:50 **Tandem MS of Synthetic Nanoparticles through Analysis of Metastable Fragments using MALDI-TOF MS with Superconducting Tunnel Junction Cryodetection**; Logan D Plath¹; Chenjie Zeng¹; Yuxiang Chen¹; Rongchao Jin¹; Mark E Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA

ThOB pm 04:10 **Ultraviolet Photodissociation in a Full-Featured Proteomics Search Engine**; Christopher Becker¹; Yong J Kil¹; Marshall W. Bern¹; Sylvester M Greer²; Jennifer S Brodbelt²; ¹Protein Metrics, San Carlos, CA; ²University of Texas at Austin, Austin, TX

2:30-4:30 pm THURSDAY

MS SOLUTIONS FOR DRUG METABOLISM CHALLENGES

Yang Yuan (Dupont Crop Protection)

Stars Ballroom 1, level 3

ThOC pm 02:30 **Direct and Accurate Quantitation of Labeled and Un-labeled Ion Species from High Resolution LC/MS Data**; Peter L Wang¹; Dawei Zhou¹; Xinping Fang¹; MING GU²; Yongdong Wang³; Jeff S. Andrews³; ¹XenoBiotic Laboratories, Inc. WuXi

AppTec Inc Plainsboro, NJ; ²Cerno Bioscience, Yardley, PA; ³Cerno Bioscience, Norwalk, CT

ThOC pm 02:50 **Understanding the Metabolism of Protein and Peptide Therapeutics by Developing a Top-Down Protein Metabolite Identification Platform**; Xiang Yu¹; Arthur Fridman¹; Kristen A Kwasnjuk¹; Ping Lu¹; Zhiling Li¹; Sherrie Xu¹; Ansu Bagchi¹; Mark T Cancilla¹; ¹Merck & Co., West Point, PA

ThOC pm 03:10 **Utilizing Tandem Mass Spectrometry for the Identification of Primary and Secondary Sulfonamide Functionalities in Protonated Analytes via Ion/Molecule Reactions**; John Kong¹; Ravikiran Yerabolu¹; Huaming Sheng¹; Weijuan Tang¹; Raghavendhar Kotha¹; Chungang Gu²; Hilkka Kenttämää¹; ¹Purdue University, West Lafayette, IN; ²AstraZeneca, Boston, MA

ThOC pm 03:30 **Software Aided Integrated Workflow for Identification of Metabolic "Soft-spots" of Macromolecular Peptides in Drug Discovery**; Asoka Ranasinghe¹; Serhiy Hnatyshyn¹; Eugene Ciccimaro¹; Celia D'Arienzo¹; Timothy Olah¹; Marshall M Siegel²; Gary Walker²; ¹Bristol-Myers Squibb Company, Princeton, NJ; ²MS Mass Spec Consultants, Fair Lawn, NJ

ThOC pm 03:50 **Toward Intact Protein Mass Spectrometry for Metabolism, Pharmacokinetic, and Toxicokinetic Study Support: Immunocapture LC-MS Methods for AlbudAb and mAb Biotherapeutics**; John Kellie; GSK, King of Prussia, PA

ThOC pm 04:10 **Novel and Widely-Applicable Platform to Uncover Pharmacologically Active Metabolites Using Metabolic Biotransformation, Affinity Selection-Mass Spectrometry, and 2D NMR Technique**; Xianshu Yang¹; Ian W Knemeyer¹; Chad Chamberlin¹; Peter J Dandliker¹; Ting Zhang²; Yong Liu²; Gary E Martin²; Huifang Yao²; Jackie Shang³; Randal M Bugianesi³; Kenneth P Ellsworth³; Lisa M Sonatore³; Peter Nizner³; Edward C Sherer²; Susan E Hill¹; Wayne M Geissler³; Roy Helmy²; Harold B Wood²; ¹Merck & Co., Boston, MA; ²Merck, Darmstadt, Germany; ³Merck & Co, Kenilworth, NJ

2:30-4:30 pm THURSDAY

AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS

Nicholas Brunelli (The Ohio State University)

Stars Ballroom 2-3, level 3

ThOD pm 02:30 **Coupling Electrochemistry with Probe Electrospray Ionization Mass Spectrometry (PESI-MS)**; Yi Cai¹; Hao Chen¹; ¹Ohio University, Athens, OH

ThOD pm 02:50 **Fundamental Studies of Inlet Ionization with Sample Introduction at Atmospheric Pressure**; Sarah Trimpin¹; Stephan Rauschenbach²; I-Chung Lu³; Casey Foley³; ¹Wayne State University, Detroit, MI; ²Max-Planck-Institute for Solid State Research, Stuttgart, Germany; ³Wayne State University, Detroit, MI

ThOD pm 03:10 **Successful Direct SPME-DBDI Coupling for Rapid, Ultrasensitive and Non-Chromatographic Analysis of Pesticides and Illicit Drugs in Complex Matrices**; Mario Francesco Mirabelli¹; Emanuela Gionfriddo²; Janusz Pawliszyn²; Renato Zenobi¹; ¹ETH Zurich, Zürich, Switzerland; ²University of Waterloo, Waterloo ON, Canada

ThOD pm 03:30 **Direct Biofluid Analysis using Hydrophobic Paper Spray Mass Spectrometry**; Deidre Damon¹; Abraham Badu-Tawiah²; ¹The Ohio State University, Columbus, OH; ²The Ohio State University, Columbus, Ohio

ThOD pm 03:50 **Back to Basics - Redesigning the DESI Sprayer for Optimal Performance in Biological Tissue Imaging;** Jocelyn Tillner¹; James McKenzie¹; Emrys A Jones^{2,1}; Steven D Pringle²; Tamas Karancsi²; Anna Mroz¹; Dipa Gurung¹; Josephine Bunch³; Ian Gilmore³; Zoltan Takats¹; ¹Imperial College, London, United Kingdom; ²Waters, Manchester, United Kingdom; ³National Physical Laboratory, Teddington, United Kingdom

ThOD pm 04:10 **Fast SAWN MS Assay for Art Restoration and Conservation studies;** Garry Corthals¹; Alina Astefanei²; Petra J Jansen²; Maarten R van Bommel²; Erik Nilsson³; Gloria Yen³; ¹University of Amsterdam, Amsterdam, ZH; ²University of Amsterdam, Amsterdam, The Netherlands; ³Deurion LLC, Seattle, WA

**2:30-4:30 pm THURSDAY
BIOMARKERS: QUANTITATIVE ANALYSIS
Matthew M. Champion (University of Notre Dame)
Stars Ballroom 4, level 3**

ThOE pm 02:30 **Disrupted Stoichiometric Relationships as Biomarkers of Altered Cellular States;** Marija Buljan¹; Tiannan Guo¹; Qing Zhong²; Ulrich Wagner²; Li Li³; Andreas Beyer³; Peter Wild²; Ruedi Aebersold¹; ¹Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; ²Institute of Surgical Pathology, University Hospital Zurich, Zurich, Switzerland; ³University of Cologne, Cologne, Germany

ThOE pm 02:50 **Understanding Biological Heterogeneity through Mass Cytometry;** Jennifer Frahm¹; Christina Loh²; Tad George²; Mark Konrad¹; Olga Ornatsky²; Daniel Majonis²; Andrei Terekidi²; Gary Impey²; ¹Fluidigm Corporation, South San Francisco, CA USA; ²Fluidigm Canada Inc., Markham, CANADA

ThOE pm 03:10 **Antibody-Independent, Deep-Dive Targeted Quantification of Proteins at Ten Picogram per Milliliter Levels in Non-Depleted Human Serum/Plasma;** Song Nie¹; Tujin Shi¹; Thomas Fillmore¹; Yuqian Gao¹; Athena A Shepmoes¹; Heather Brewer¹; Wei-jun Qian¹; Karin D Rodland¹; Richard D Smith¹; Tao Liu¹; ¹Biological Sciences Division and Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

ThOE pm 03:30 **Mass Spectrometry Based Identification and Quantitation of Maturation Stage Specific Surface Markers of Human Stem Cell Derived Cardiomyocytes;** Matthew Waas¹; Erin Kropp¹; Alyssa Nycz¹; Chelsea Fujinaka¹; Rebekah Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI

ThOE pm 03:50 **Discovery and Quantitative Metabolomics to Characterize Metabolites of Bacterial Origin as Biomarkers for Cystic Fibrosis;** Jace W Jones¹; Angela Nguyen¹; Bennett Giardina¹; Luke Brewer¹; Angela Wilks¹; Amanda Oglesby-Sherrouse¹; Maureen Kane¹; ¹University of Maryland, School of Pharmacy Baltimore, MD

ThOE pm 04:10 **Quantifying Concentrations of Molecules in Live Single Cells using the Single-probe MS Technique;** Ning Pan¹; Wei Rao¹; Haiqing Yu¹; Naga Rama Kothapalli¹; Mei Sun¹; Anthony Burgett¹; Zhibo Yang¹; ¹University of Oklahoma, Dept. of Chem & Biochem Norman, OK

**2:30-4:30 pm THURSDAY
INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION
Natalie Castellana (Digital Proteomics LLC)
Hemisfair Ballroom 3, level 3**

ThOF pm 02:30 **A Graph-based Method for Proteoform Identification and Quantification by Top-down Multiplexed Tandem Mass Spectra;** Zhu Kaiyuan¹; Xiaowen Liu²; ¹Indiana University, Bloomington, IN; ²Indianapolis, IN

ThOF pm 02:50 **High Quality Estimation of False Discovery Rate for Proteoform Identification with Top Down Proteomics;** Richard Leduc¹; Daniel Shams²; ³Ryan T Fellers¹; Bryan Early¹; Joseph Greer¹; David Schwab³; Neil L Kelleher^{1,4,5,6}; ¹Proteomics Center of Excellence, Northwestern University, Evanston, IL; ²Interdisciplinary Biological Sciences, Northwestern University, Evanston, IL; ³Department of Physics and Astronomy, Northwestern University, Evanston, IL; ⁴Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; ⁵Department of Chemistry, Northwestern University, Evanston, IL; ⁶Department of Molecular Biosciences, Northwestern University, Evanston, IL

ThOF pm 03:10 **Open-pNovo: de novo Peptide Sequencing with Thousands Types of Protein Modifications;** Hao Yang¹; Hao Chi¹; Wen-Jing Zhou¹; Wen-Feng Zeng¹; Kun He¹; Chao Liu¹; Rui-Xiang Sun¹; Si-Min He¹; ¹Institute of Computing Technology, CAS, Beijing, China

ThOF pm 03:30 **Optimized Open Modification Spectral Library Searching using Approximate Nearest Neighbor Techniques;** Wout Bittremieux¹; Dirk Valkenborg²; Kris Laukens³; ¹University of Antwerp, Antwerp; ²VITO, Mol, Belgium; ³University of Antwerp, Antwerp, Belgium

ThOF pm 03:50 **Sifting through Swarms of Spectra: Lessons Learned Identifying Proteins across 11,782 Affinity-Purification Mass Spectrometry Analyses;** Edward L. Huttlin¹; Joao A Paulo¹; Raphael J. Bruckner¹; Lily Ting¹; Wade Harper¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA

ThOF pm 04:10 **Building Comprehensive Peptide Spectral Libraries at Repository Scale;** Mingxun Wang¹; Jian Wang¹; Anne-Claude Gingras²; Nuno Bandeira¹; ¹UCSD, San Diego, CA; ²Lunenfeld Tanenbaum Research Institute, Toronto, Canada

**2:30-4:30 pm THURSDAY
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Daniel Amador-Noguez (University of Wisconsin-Madison)
Hemisfair Ballroom 2, level 3**

ThOG pm 02:30 **A Quantitative Positive/Negative Ion Switching Method for Shotgun Lipidomics via High Resolution LC-MS/MS from any Biological Source;** Min Yuan¹; Ying Xu¹; Susanne Breitkopf¹; Stephane Ricoult²; John M Asara¹; ¹Beth Israel Deaconess Medical Center, Boston, MA; ²Harvard School of Public Health, Boston, MA

ThOG pm 02:50 **Lipidomic Imaging with a New Hybrid 3D SIMS Molecular Imaging Instrument;** Melissa K Passarelli¹; Alexander Pirk²; Rudolf Moellers²; Ewald Niehuis²; Alexander A Makarov³; Henrik Arlinghaus²; Rasmus Havelund¹; Paulina Rakowska¹; Alan Race¹; Alex Shard¹; Andy West⁴; Stevan Horning³; Peter Marshall⁴; Morgan Alexander⁵; Colin Dallery⁴; Ian Gilmore¹; ¹National Physical Laboratory, Teddington, United Kingdom; ²ION-TOF GmbH, Munster, Germany; ³Thermo Fisher Scientific, Bremen, DE; ⁴GlaxoSmithKline, Stevenage, UK; ⁵University of Nottingham, Nottingham, UK

THURSDAY AFTERNOON ORAL SESSIONS

- ThOG pm 03:10 **Electron-induced Dissociation (EID) of Lipids: Diagnostic Product Ions for Confident Identification of Isomers;** Jace W. Jones¹; Claire Louise Carter¹; Maureen A Kane¹; ¹University of Maryland, School of Pharmacy Baltimore, MD
- ThOG pm 03:30 **Broad Characterization of Isomeric Lipids by High-Resolution Differential Ion Mobility Separations with Tandem Mass Spectrometry;** Rinat R Abzalimov¹; Andrew Bowman²; Alexandre A Shvartsburg²; ¹City University of New York - Advanced Science Research Center, New York City, NY; ²Wichita State University, Wichita, KS
- ThOG pm 03:50 **Nano-DESI Imaging of Lipids and Metabolites in Developing Lung;** Son N. Nguyen¹; Ryan L Sontag¹; Jennifer E Kyle¹; Sydney E Dautel¹; Thomas O Metz¹; Richard A Corley¹; Charles K Ansong¹; Mathew Thomas¹; James Carson²; Julia Laskin¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Texas at Austin, Austin, TX
- ThOG pm 04:10 **In depth Sphingomyelin and Triacylglycerol Structure Identification using Electron Impact Excitation of Ions from Organics (EIEIO) and Mass Spectrometry;** Takashi Baba¹; Larry J Campbell¹; Yves J C LeBlanc¹; Paul RS Baker²; ¹SCIEX, Concord ON, Canada; ²SCIEX, Redwood City, CA

**2:30-4:30 pm THURSDAY
HYDROGEN-DEUTERIUM EXCHANGE MS
Sheena D'Arcy (University of Texas at Dallas)
Hemisfair Ballroom 1, level 3**

- ThOH pm 02:30 **HX-MS Epitope Mapping of a Ricin Toxin Chain A Double Mutant (RTA*);** Ronald Toth¹; Siva Krishna Angalakurthi¹; John Hickey¹; Sangeeta Joshi¹; Charles Russell Middaugh¹; Greta Van Slyke²; Nicholas Mantis^{2,3}; David Volkin¹; David Weis⁴; ¹Department of Pharmaceutical Chemistry and Macromolecule and Vaccine Stabilization Center; University of Kansas, Lawrence, KS; ²Division of Infectious Disease, Wadsworth Center, New York State Department of Health, Albany, NY; ³Department of Biomedical Sciences, University at Albany School of Public Health, Albany, NY; ⁴Department of Chemistry and R. N. Adams Institute for Bioanalytical Chemistry; University of Kansas, Lawrence, KS
- ThOH pm 02:50 **The Role of Conformational Dynamics in Differing Activity and Substrate Specificity amongst Isozymes;** Andrew Fairman¹; Peter Sidhu¹; David Josephy²; Derek Wilson¹; ¹York University, Toronto, Canada; ²University of Guelph, Guelph, Canada
- ThOH pm 03:10 **Structural basis for the formation and function of the complement effector protein iC3b;** Malvina Papanastasiou¹; Sophia Koutsogiannaki¹; Yiannis Sarigiannis¹; Daniel Ricklin¹; John D. Lambris¹; ¹Dept. Pathology & Lab. Medicine, Perelman School of Medicine, UPENN, Philadelphia, PA
- ThOH pm 03:30 **A New Automation Platform Provides Significant Improvements in Both the Capacity and Flexibility of the HDX-MS Experiment;** Ruben Haro¹; Alfonso Espada¹; Manuel Molina-Martin¹; Jesus Castanon¹; Bruce D Pascal²; Pat Griffin²; Jeffrey A Dodge³; Michael Chalmers³; ¹Eli Lilly and Company, Alcobendas, SPAIN; ²The Scripps Research Institute, Jupiter, FL; ³Eli Lilly and Company, Indianapolis, IN

- ThOH pm 03:50 **Intramolecular Interactions in Heme Oxygenase 2 in the Presence and Absence of Lipid Membranes;** Brent A Kochert¹; Angela S Fleischhacker²; Stephen W Ragsdale²; John R Engen¹; ¹Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; ²Department of Chemistry, University of Michigan, Ann Arbor, MI
- ThOH pm 04:10 **The Analytical Potential of HDXMS in Providing Localized Structural Dynamics Insight to Each Subunits of an Asymmetric Non-Crystallizable Protein Homodimer;** Morten Beck Trelle¹; Alice Østergaard²; Jeppe Buur Madsen¹; Shona Pedersen²; Søren Risom Kristensen²; Thomas J.D. Jørgensen¹; ¹University of Southern Denmark, Odense, Denmark; ²Department of Clinical Medicine, Aalborg University Hospital, Aalborg, Denmark, Aalborg, Denmark

4:45 - 5:00 PM

PLENARY LECTURE

**Vicki Wysocki (The Ohio State University) presiding
Hall 1, level 1**



More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds

William Bialek
Princeton University

6:30 – 9:00 PM, THURSDAY

CLOSING EVENT

BRISCOE WESTERN ART MUSEUM

Ticket is required.



ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:00 - 2:30 PM.

MONDAY POSTERS

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

Antibodies & Antibody Drug Conjugates (Intact and Characterization).....	001 - 020
Biomolecular Structure Analysis: Covalent Labeling and Related Software.....	021 - 039
Carbohydrates.....	040 - 055
Data Independent Acquisition.....	056 - 070
Diagnostic Clinical Chemistry (Applications).....	071 - 094
Drug and Metabolite Analysis: Novel Approaches for Dried Biological Samples.....	095 - 103
Energy: Hydrocarbon and Petrochemical (Ultra Hi Res).....	104 - 122
Environmental Analysis: General (Part 1).....	123 - 147
Environmental Analysis: Pharmaceuticals and Pesticides.....	148 - 176
Epigenetic Modifications.....	177 - 194
High Mass Accuracy/High Performance MS Applications.....	195 - 210
Imaging MS: Instrumentation.....	211 - 231
Imaging MS: Sample Preparation.....	232 - 243
Imaging MS: Software.....	244 - 249
Informatics: Metabolomics.....	250 - 264
Informatics: Multiomics Integration.....	265 - 280
Instrumentation: New Concepts.....	281 - 302
Intact Proteins.....	303 - 319
Ion Activation/Dissociation.....	320 - 340
Ion Mobility: Applications (Other/Instrumentation).....	341 - 373
Ion Molecule, Ion/Ion, Ion/Electron Interactions.....	374 - 398
Ion Spectroscopy.....	399 - 411
LC-MS: Chromatography and Software (Part 1).....	412 - 440
Lipids: General.....	441 - 456
Metabolomics: General.....	457 - 495
Microorganisms: Identification and Characterization.....	496 - 517
Phosphopeptides: Enrichment Methods.....	518 - 529
Polymers.....	530 - 548
Proteins: General and Membrane.....	549 - 571
Proteins: PTMs (Part 1).....	572 - 596
Proteomics: Clinical Applications (Applied Proteomics).....	597 - 621
Proteomics: Quantitative.....	622 - 650
Small Molecules: Qualitative Analysis.....	651 - 680
Systems Biology (Multiomics and Other).....	681 - 707
Top Down Protein Analysis (Applications).....	708 - 727

TUESDAY POSTERS

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

Antibodies & Antibody Drug Conjugates (Separations).....	001 - 028
Biomarkers: Quantitative Analysis (Part 1).....	029 - 054
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling (Cross-Linking).....	055 - 075
Data Independent Acquisition (SWATH).....	076 - 095
Diagnostic Clinical Chemistry (General).....	096 - 112
Drug Discovery/DMPK/ADME (Applications).....	113 - 129
Drug Metabolism: Qualitative and High Throughput Analysis.....	130 - 144
Energy: Hydrocarbon & Petrochemical (Hi Res and Nominal).....	145 - 163
Environmental Analysis: General (Part 2).....	164 - 188
FAIMS and DMS.....	189 - 209
Food Safety (Pesticides in Food).....	210 - 235
Food"omics" MS Characterization of Food and Nutritional Supplements (Part 1).....	236 - 250
Forensics (Part 1).....	251 - 278
Glycoproteins.....	279 - 296
High Mass Accuracy/High Performance MS Methods and Developments.....	297 - 312
Imaging MS: Disease Markers.....	313 - 344
Imaging MS: Pharmaceutical Applications.....	345 - 363
Informatics: Peptide ID and Quantification.....	364 - 391
Instrumentation: General.....	392 - 416
Instrumentation: New Developments in Mass Analyzers.....	417 - 442
Ion Mobility: Applications (Proteins & Peptides).....	443 - 470
LC-MS: Chromatography and Software (Part 2).....	471 - 498
Lipids: ID and Structural Analysis.....	499 - 518
Metabolomics: Sample Preparation.....	519 - 529
Metabolomics: Untargeted Metabolite Profiling (Cells/Plants).....	530 - 557
Nucleic Acids.....	558 - 582
Peptides: PTM Identification.....	583 - 605
Phosphopeptides: Quantitative Analysis.....	606 - 623
Proteins: Complexes/Non-covalent Interactions.....	624 - 659
Proteomics: Clinical Applications (Development toward Clinical Application).....	660 - 681
Proteomics: Infectious Diseases.....	682 - 702
Proteomics: Quantitative (Application Biological Research).....	703 - 727
Small Molecules: Quantitative Analysis (Animal, Plant/Insect, and Methodology).....	TP 728 - 762
Top Down Protein Analysis (Methodology).....	TP 763 - 775



POSTER OVERVIEW

ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:30 - 2:30 PM.

WEDNESDAY POSTERS

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

Ambient Ionization: Fundamentals and Instrumentation (Probes, Paper Spray, DESI/ESI, Tissue/Tools).....	001 - 029
Antibodies & Antibody Drug Conjugates (Sequencing, Modifications & Hi Res).....	030 - 061
Biomarkers: Discovery (Part 1).....	062 - 088
Biomarkers: Quantitative Analysis (Part 2).....	089 - 116
Carbohydrates (Glycans).....	117 - 138
Disease Biomarkers	139 - 153
Drug Discovery/DMPK/ADME (General).....	154 - 177
Energy: Biofuels and Algae	178 - 189
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THURSDAY POSTERS

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

Ambient Ionization: Fundamentals and Instrumentation (Dart/Plasma, Laser, SAWN).....	001 - 030
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Set up all Monday posters 7:30 – 8:00 am
Odd-numbered posters present 10:30 am – 1:00 pm
Even-numbered posters present 12:00 – 2:30 pm
 Remove all Monday posters 7:30 – 8:00 pm

Antibodies & Antibody Drug Conjugates (Intact and Characterization).....	001 - 020
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Informatics: Multiomics Integration.....	265 - 280
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Ion Mobility: Applications (Other/Instrumentation).....	341 - 373
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Lipids: General.....	441 - 456
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Proteins: General and Membrane.....	549 - 571
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Proteomics: Clinical Applications (Applied Proteomics).....	597 - 621
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ANTIBODIES & ANTIBODY DRUG CONJUGATES (INTACT & CHARACTERIZATION) **001 - 020**

- MP 001 **Integrating Intact, Reduced and IdeS Approaches for Rapid Differentiation and Verification of Monoclonal Antibodies Using Liquid Chromatography Q-Exactive Mass Spectrometry;** Lianji Jin; FDA, Cincinnati, OH
- MP 002 **Online Separation and Characterization of intact IgG Fabs Using Ultra Performance Liquid Chromatography Coupled with Top-down Mass Spectrometry;** Zhe Wang; Kenneth Smith²; Si Wu¹; ¹University of Oklahoma, Dept. of Chem & Biochem Norman, OK; ²Oklahoma Medical Research Foundation, Oklahoma City, OK
- MP 003 **Evaluation of Different Immunocapture Platforms for Antibody-Conjugate Drug Quantification;** Ling Xu; Shaoxia Yu²; Jing-Tao Wu³; Mark Qian³; ¹Millennium Pharma, Cambridge, MA; ²Takeda Pharmaceutical International Inc., Cambridge, MA; ³Takeda Pharmaceuticals International Inc., Cambridge, MA
- MP 004 **Intact Mass Analysis of Antibody-drug conjugates (ADCs) as a Tool to Measure Payloads of Linked Cytotoxic Drugs;** Joe Shambaugh¹; Cassandra Wigmore²; Maurizio Bronzetti¹; David Bush¹; Arnd Brandenburg²; Peter Haber³; ¹Genedata Inc, Lexington, MA; ²Genedata AG, Basel, Switzerland; ³Genedata GmbH, Munich, Germany

- MP 005 **Characterization of Bispecific Antibodies Using Mass Spectrometry during Cell Line Development is Critical for an Optimized Final Drug Product;** Michael Bacica¹; Jon R Fitchett¹; Stephen J Demarest¹; Xiufeng Wu¹; Robert Peery²; Bryan Jones¹; ¹Lilly Biotech Center-San Diego, San Diego, CA; ²Lilly BioTDR, Indianapolis, IN
- MP 006 **Developability Assessment of Multispecific Biopharmaceuticals;** Kadir Ilker Sen¹; Eric Beil¹; Hirsh Nanda¹; Andrew Mahan¹; Darryl Davis¹; ¹Janssen Research and Development, Spring House, PA
- MP 007 **Monitoring the Critical Quality Attributes of Antibody Drug conjugates (ADCs) as Part of Biosimilar Development: Case Studies of ado-trastuzumab emtansine;** Liuxi Chen¹; Min Du¹; Henry Y Shion¹; Ying-Qing Yu¹; Lan Wang²; Kai Gao²; Weibin Chen¹; ¹Waters Corporation, Milford, USA; ²National Institutes for food and drug control, Beijing, CN
- MP 008 **Detection of an Amino Acid Sequence Variant as a Function of Cell Line Stability in a Model Antibody;** Sylvia Jozwiak¹; James Graham¹; ¹Lonza, Slough, UK
- MP 009 **Assessment of Critical Parameters for the Mass Spectrometric Evaluation of the Drug-to-Antibody Ratio in Antibody-Drug Conjugates;** Neil Hershey¹; Shiyue Zhou²; Yunping Huang¹; Hangtian Song¹; Hui Wei¹; Jacob Bongers¹; Richard Ludwig¹; Li Tao¹; Tapan Das¹; ¹Bristol-Myers Squibb, Hopewell, NJ; ²Texas Tech University, Lubbock, Texas
- MP 010 **An Automated Quantitative Mass Spectrometry Assay to Determine Intra-Cellular Retention Kinetics of Antibiotic Released from Anti-Staphylococcus Aureus Antibody-Antibiotic Conjugate;** Hilda Hernandez-Barry¹; Kimberly Kajihara²; Daniel Tran²; Martine Darwish²; Byoung-Chul Lee²; Richard Vanden²; Leanna Staben²; Thomas Pillow²; Wouter Hazenbos²; Kelly Loyet²; ¹Genentech, South San Francisco, CA; ²Genentech Inc, South San Francisco, CA
- MP 011 **An Automated Sample Extraction and Processing Method Combining Ligand Binding and Mass Spectrometry Analysis for Biotherapeutics Quantitation;** Ian Moore; SCIEX, Concord, ON
- MP 012 **A Comprehensive Mass Spectrometric Workflow for Characterizing Therapeutic Antibodies;** Alicia Bielik¹; Paula Magnelli¹; Beth McLeod¹; Colleen McClung¹; Beth Paschal¹; Cristian I Ruse¹; Xiaofeng Shi¹; Ellen Guthrie¹; ¹New England Biolabs, Ipswich, MA
- MP 013 **Drug-to-Antibody Ratio Determination for Antibody-Drug Conjugates in Serum Enabled by a Sample Preparation Platform that Automates Affinity Purification and Deglycosylation;** Jing Chen¹; Maryann Shen²; Steve Murphy¹; ¹Agilent Technologies, Inc. Madison, WI; ²Agilent Technologies, Santa Clara, CA
- MP 014 **Platform Method for Identity and Characterization of Therapeutic Monoclonal and Bispecific Antibodies by Intact and Reduced Mass Spectrometry;** Richard Seipert¹; Lisa Patterson²; George Tsui²; Chris Yu²; ¹Genentech, South San Francisco, CA; ²Genentech Inc, South San Francisco, CA
- MP 015 **A Tag-free Collisionally-Induced Fragmentation Technique Applied to Studies of Antibody-drug Conjugate Lysosomal Processing;** Andrew Bessire¹; Chakrapani Subramanyam²; My-Hahn Lam³; Frank Loganzo³; T. Eric Ballard²; ¹Pfizer, Inc., Groton, CT; ²Pfizer, Groton, CT; ³Pfizer Oncology-Rinat R&D, Pearl River, NY
- MP 016 **Strategy to Rapidly and Comprehensively Characterize Innovator Biologics and their Biosimilars via Stress Testing Studies;** Esthelle Hoedt¹; St John Skilton²; Yong J Kil³; Eric Carlson⁴; Chris Becker³; Beatrix M Ueberheide¹; ¹NYU School of Medicine, New York City, NY; ²Protein Metrics, Hopkinton, MA; ³Protein Metrics, San Carlos, CA; ⁴Protein Metrics Inc., San Carlos, CA



- MP 017 **Method Development for the Detection and Quantitation of Monomethyl Auristatin F (MMAF) in Cell Culture Media**; Maria Christina Malinao¹; Melissa M. Williams¹; Cody Warhurst¹; Julien Dugal-Tessier¹; Josh T. Snyder¹; Brian Mendelsohn¹; Hui Zhao¹; Sara Gulesserian¹; Hosein Kouros-Mehr¹; Kendall Morrison¹; ¹Agensys, Inc. Santa Monica, CA
- MP 018 **In-Depth Characterization of Monoclonal Antibodies with a Single Experiment and Fully Automated Data Analysis**; Paul Taylor¹; Johnathan Krieger¹; Qixin Liu²; Mingjie Xie²; Lian Yang^{2,3}; Bin Ma³; ¹Hospital for Sick Children, Toronto, Canada; ²Rapid Novor Inc., Waterloo ON, Canada; ³University of Waterloo, Waterloo ON, Canada
- MP 019 **Antibody Variable Domains as Intramolecular Luciferase Inhibitors for the Generation of Proteolysis-Activated Biosensors**; Lining Zhu¹; Teresa Hong¹; Nicola McNiven¹; Markus Kalkum¹; ¹City of Hope, Duarte, CA
- MP 020 **Novel Strategy Based on Dual Enrichment and Double Lists for Characterization of Host Cell Proteins**; Zheng-Xiang Zhang¹; Jimmy Chan¹; Shuai Zuo¹; Tao Bo¹; Rong An¹; ¹Agilent Technologies (China) Limited, Beijing, China

BIOMOLECULAR STRUCTURE ANALYSIS: COVALENT LABELING AND RELATED SOFTWARE

021 - 039

- MP 021 **Using High Resolution Structural Analysis to Determine if FPOP Modification Perturbs Native Protein Structure**; Emily Hart¹; Lisa M Jones¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- MP 022 **Extension of the FPOP Method for Oxidative Modification in Live Tissue**; Jessica Arlett Espino¹; Anthony J Baucum¹; Lisa M Jones²; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²Indiana University Purdue University Indianapolis, Indianapolis, IN
- MP 023 **Epitope Map of Malarial Antigen PvDBP revealed by Fast Photochemical Oxidation of Proteins (FPOP)**; Manolo David Plasencia¹; Yining Huang¹; Henry W Rohrs¹; Edwin Chen²; Nichole D. Salinas²; Niraj H. Tolia²; Michael L Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- MP 024 **The Application of "Droplet-Like" Methods to FPOP**; Don L. Rempel¹; Supratik Dutta²; Ben Niu²; Yining Huang²; Manolo Plasencia²; Michael Gross²; ¹Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO; ²Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO
- MP 025 **Normalization of High Resolution Hydroxyl Radical Protein Footprinting Data to Protein Structural Properties**; Boer Xie¹; Amika Sood¹; Robert J Woods¹; Joshua S. Sharp²; ¹University of Georgia, Athens, GA; ²University of Mississippi, University, MS
- MP 026 **Automated Hydroxyl Radical Protein Footprinting for the Determination of Biopharmaceutical Protein Conformation**; Franklin E. Leach III¹; Ron Orlando²; Joshua S Sharp³; ¹Photochem Technologies, Athens, GA; ²Complex Carbohydrate Research Center UGA, Athens, GA; ³School of Pharmacy, University of Mississippi, Oxford, MS
- MP 027 **Develop Isotope-encoded Photoaffinity Footprinting Reagent for Structural Mass Spectrometry Studies**; Ming Cheng¹; Michael L Gross¹; ¹Washington University in St. Louis, St. Louis, MO
- MP 028 **Exploring the Peroxidase Activation and Deactivation of Cytochrome C by Heme-Catalyzed Oxidative Labeling and ESI-MS**; Victor Yin¹; Lars Konermann¹; ¹Western University, London, Canada

- MP 029 **Comprehensive Measurement of Protein Dynamics in Complex Environments Using Footprinting Mass Spectrometry with Inexpensive MS2 Quantification of Labeled Cysteines**; Jenna Gray Caldwell¹; Pehr A. B. Harbury¹; ¹Stanford University School of Medicine, Palo Alto CA
- MP 030 **Using Covalent Labeling and Mass Spectrometry to Study b-2-Microglobulin-Inhibitor Binding Sites**; Tianying Liu¹; Richard W Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- MP 031 **Towards an Improved Understanding of Diazirine Labeling for Structural Mass Spectrometry Applications**; Daniel Ziemianowicz¹; Chris Etienne²; David Schriemer¹; ¹University of Calgary, Calgary, Canada; ²Thermo Fisher Scientific, Rockford, IL
- MP 032 **Characterisation Proteolytic Process by Protein N-Terminal Derivatisation in- Gel Using MS-Based Approach in Drosophila**; Nina Guillaumot¹; Florian Veillard²; Jean-Marc Reichhart²; Alain Van dorselaer¹; Christine Schaeffer-Reiss¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, Université de Strasbourg, CNRS, UMR7178, Strasbourg, Strasbourg, France; ²Institut de Biologie Moléculaire et Cellulaire, IBMC, Université de Strasbourg, CNRS UPR 9022, Strasbourg, Strasbourg, France
- MP 033 **Covalent Labeling Denaturation Mass Spectrometry for Sensitive Localized Higher Order Structure Comparisons**; James A. Madsen¹; Yan Yin¹; Jing Qiao¹; Vanessa Gill¹; Kutralanathan Renganathan¹; Wing-Yee Fu¹; Stephen Smith¹; James Anderson¹; ¹Momenta Pharmaceuticals, Cambridge, MA
- MP 034 **Xilmass: A New Approach Towards the Identification of Cross-Linked Peptides**; Sule Yilmaz^{1,2,3}; Friedel Drepper⁴; Maša Černič⁵; Kris Gevaert^{1,7}; Anastassios Economou⁸; Bettina Warscheid^{4,5}; Lennart Martens^{1,7,10}; Elien Vandermarliere^{1,7,10}; ¹Department of Biochemistry, Ghent University, Ghent, BELGIUM; ²Medical Biotechnology Center, Ghent, BELGIUM; ³Bioinformatics Institute Ghent, Ghent, BELGIUM; ⁴Department of Biochemistry and Functional Proteomics, Institute of Biology II, Faculty of Biology, University of Freiburg, Freiburg, Germany; ⁵BIOSS Centre for Biological Signaling Studies, University of Freiburg, Freiburg, Germany; ⁶Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins, Ljubljana, Slovenia; ⁷Medical Biotechnology Center, VIB, Ghent, BELGIUM; ⁸Laboratory of Molecular Bacteriology, Rega Institute for Medical Research, Department of Microbiology and Immunology, KULeuven, Leuven, BELGIUM; ⁹Institute of Molecular Biology and Biotechnology-FoRTH, Department of Biology – University of Crete, Iraklio, Crete, Greece; ¹⁰Bioinformatics Institute Ghent, Ghent University, Ghent, BELGIUM
- MP 035 **Crosslinkers with Isotope-Coding and Cleavable Spacers Improve Peptide Crosslink Identification by a Semi-Supervised Machine Learning Algorithm**; Karl A T Makepeace¹; Evgeniy V Petrochenko¹; Christoph H. Borchers^{2,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 036 **A Simple Approach for Creating Protein Structural Models Based on Cross-Linking Data**; Zsuzsanna Orban-Nemeth¹; Evelyn Rampler¹; Thomas Stranzl¹; David Maria Hollenstein²; Otto Hudecz³; Peter Schloegelhofer⁴; Karl Mechtler^{1,3}; ¹Institute of Molecular Pathology, Vienna, Austria; ²Department of Biochemistry and Cell Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria; ³Institute of Molecular Biotechnology, Austrian Academy of Sciences, Vienna, Austria; ⁴Department



of Chromosome Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria

- MP 037 **CX-Circos: A Web-Based Tool for Visualization and Analysis of Chemical Crosslinking Data;** Junjie Wang¹; Yi Shi¹; Brian T. Chait¹; ¹Rockefeller University, New York, NY
- MP 038 **In Cell Protein Footprinting Coupled with Mass Spectrometry to Probe Protein Conformational Change;** Maissa M Gaye¹; Lisa Jones¹; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN
- MP 039 **High-throughput Mass Spectrometric Analysis of Covalent Protein-inhibitor Adducts, Monoclonal Antibodies and ADCs: A Complete Workflow;** Tisha San Miguel¹; Jelly Netirojjanakul¹; Rowe Todd¹; Onea Daniel¹; Victor Cee¹; Arvedson Tara¹; McCarter John¹; Campuzano Iain¹; ¹Amgen, Inc., Thousand Oaks, CA

CARBOHYDRATES 040 - 055

- MP 040 **Quantifying Cyclodextrin-Drug Interactions by ESI-MS;** Emma-Dune Leriche¹; Ping Zhang²; Aixia Wang²; Yuyu Yao¹; Chang-Chun Ling²; Elena N Kitova¹; John S Klassen¹; ¹University of Alberta, Edmonton, Canada; ²University of Calgary, Calgary, Canada
- MP 041 **Identification and Relative Quantification C-mannosylation of Interleukin 6 (IL-6) using Liquid Chromatography-tandem Mass Spectrometry;** Anhdao Darcy; Abbvie Bioresearch Center, Worcester, MA
- MP 042 **Development of Negative Mode Free Radical Activated Glycan Structure Elucidation Reagents;** Jinshan Gao¹; Nikunj Desai¹; Jungeun Lee¹; ¹Montclair State University, Montclair, NJ
- MP 043 **Carbohydrate Analysis using Gas Chromatography Vacuum Ultraviolet Spectroscopy in Comparison with Gas Chromatography Mass Spectrometry;** Jamie Schenk¹; Xiaojian Mao¹; Jonathan Smuts²; Gabe Nagy³; Nicola L. B. Pohl³; Phillip Walsh²; Peter Kroll¹; Kevin A Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²VUV Analytics, Inc., Cedar Park, TX; ³Indiana University, Bloomington, IN
- MP 044 **Understanding the Reaction Products of Methanolysis and Butanolysis of Heparan Sulfate;** Marten F. Snel¹; Paul J Trim²; John J Hopwood²; Qi Qi He³; Vito Ferro³; ¹South Australian Health and Medical Research Institute, Adelaide, South Australia; ²LDRU, Nutrition and Metabolism Theme, South Australian Health and Medical Research Institute, Adelaide, Australia; ³School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Australia
- MP 045 **LC-MS Analysis of the Complete Molecular Weight Distribution of Low Molecular Weight Heparins;** Yuewei Sheng¹; Chun Shao¹; Kshitij Khatri¹; Joseph Zaia²; ¹Boston University School of Medicine, Boston, MA; ²Boston University, Boston, MA
- MP 046 **Size-Selective Controlled Heparin Depolymerization to Obtain Heparin Oligosaccharides;** Sandeep K Misra¹; Joshua S Sharp¹; ¹Dept of Biomolecular Sciences, University of Mississippi, Oxford, MS
- MP 047 **Oxidation of Glucose at Gold Nanoparticles and Mass Spectrometric Product Analysis;** Marilyn Wooten¹; Wendell P. Griffith²; Sushma Karra²; Waldemar Gorski²; ¹Trinity University, San Antonio, TX; ²University of Texas at San Antonio, San Antonio, TX
- MP 048 **Study of Rearrangement Products in Collision-Induced Dissociation and Surface-Induced Dissociation of Oligosaccharides and Glycoconjugates;** Forouzan Aboufazel¹; Eric D Dodds¹; ¹University of Nebraska-Lincoln, Lincoln, NE

- MP 049 **Single Stage Tandem Mass Spectrometry Assignment of the C-5 Uronic Acid Stereochemistry in Heparan Sulfate Tetrasaccharides Using Electron Detachment Dissociation;** Isaac Agyekum¹; Chengli Zong^{2,3}; Geert-Jan Boons^{2,3}; Jon Amster²; ¹University of Georgia, Chemistry Department, Athens, GA; ²University of Georgia, Chemistry Department Athens, GA; ³CCRC, University of Georgia Athens, GA
- MP 050 **Mass Spectrometric Quantification of Cell Wall Composition Differences in Enterococcus Using Stable Isotope Labeling by Amino Acids;** James Chang¹; Ashley Wallace¹; Erin Foster¹; Alex Guinn¹; Sung Joon Kim¹; ¹Baylor University, Waco, TX
- MP 051 **High Resolution CESI-MS Analysis of APTS-Labeled N-Glycans of Biopharmaceutical Interest;** Fonslow Bryan; Marton Szigeti¹; Andras Guttman²; ¹University of Debrecen, Debrecen, Hungary; ²AB Sciex, San Diego, CA
- MP 052 **Probing Carbohydrate Isomerism through Transition Metal Ion Addition, Gas-Phase Ion Chemistry, and Collision-Induced Dissociation;** Katherine Schumacher¹; Yuting Huang¹; Lauren Petrosh¹; Eric D Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- MP 053 **ESI-TOF-MS Study of Carbohydrate Interaction with Metal Complexes with Carboxylate-Rich Ligand;** Fangzhi Yan¹; Christopher D. Stewart¹; Stephan B. H. Bach¹; Wendell P Griffith¹; Ghezai T. Musie¹; ¹University of Texas at San Antonio, San Antonio, TX
- MP 054 **Fragmentation of Derivatized and Non-Derivatized Metal-Adducted Oligosaccharides;** Ranelle Schaller-Duke; The University of Alabama, Tuscaloosa, AL
- MP 055 **A Novel Method for High-Throughput Analysis of Bioactive Oligosaccharides;** Randall Robinson¹; Daniela Barile¹; ¹University of California, Davis, Davis, CA

DATA INDEPENDENT ACQUISITION 056 - 070

- MP 056 **Advances in Targeted Omics Quantitation Using a Novel Scanning Quadrupole DIA Method;** Chris Hughes¹; Keith Richardson¹; Jason Wildgoose¹; Martin R Green¹; Richard Chapman¹; Arkadiusz Grzyb¹; Praveen Harapanahalli¹; Kirsten Craven¹; ¹Waters, Wilmslow, United Kingdom
- MP 057 **Optimisation of Data Independent Acquisition (DIA) Data Extraction for Proteome Quantification;** Gauthier Husson¹; Alvaro Sebastian Vaca Jacome¹; Maxime Eveque¹; Christine Carapito¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO), IPHC, Strasbourg University, CNRS, UMR7178, Strasbourg, France
- MP 058 **Improved Multiplexed Data Independent Acquisition: Sensitivity, Dynamic Range, and Full-Spectrum Demultiplexing;** Jarrett Egerton¹; Ying Sonia Ting¹; Philip M Remes²; Romain Hugué²; Derek Bailey²; Michael Senko²; Vlad Zabrouskov²; Michael J MacCoss¹; ¹Univ of Washington, Seattle, WA; ²Thermo Fisher Scientific, San Jose, CA
- MP 059 **Analytical Validation of a Data-Independent Acquisition Mass Spectrometry Workflow for Quantification and Identification of Myofibrillar Proteoforms in Cardiac Biopsies;** Irene van den Broek¹; Irina Tchernyshyov¹; Vidya Venkatraman¹; Giulio Agnetti^{2,3}; Amol Prakash⁴; Scott Peterman⁵; Jennifer E Van Eyk¹; ¹Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; ²Division of Cardiology, Johns Hopkins University School of Medicine, Baltimore, MD; ³Department of Biomedical and Neuromotor Sciences, University of Bologna, Bologna, Italy; ⁴Optys Tech Corporation, Brighton, MA; ⁵Thermo Fisher Scientific, Cambridge, MA



- MP 060 **Computational Workflows to Improve DIA Data Analysis Without Reference Libraries for Quantitative Proteomics and PTM Analysis;** Jesse Gerard Meyer¹; Birgit Schilling¹; Samir Softic²; C. Ronald Kahn²; Bradford W Gibson¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Joslin Diabetes Center and Harvard Medical School, Boston, MA
- MP 061 **Evaluation of the Efficacy of Data-Independent Acquisition Using Hyper Reaction Monitoring in Quantitative Proteome Profiling of Diverse Species;** Jing Wang¹; Jeong-Jin Park¹; David R Gang¹; ¹Washington State University, Pullman, WA
- MP 062 **Data Independent Infrared Multiphoton Dissociation for Selective Identification of Cysteine Oxidized Peptides;** Nicholas Borotto¹; Phillip McClory¹; Jaimeen Majmudar¹; Brent Martin¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI
- MP 063 **Effect of Peptide Assay Library Size and Composition in Targeted Data Independent Acquisition-Mass Spectrometry Analyses;** Vidya Venkatraman¹; Sarah Parker¹; Jennifer E Van Eyk¹; ¹Advanced Clinical Biosystems Research Institute, Los Angeles, CA
- MP 064 **Spectral Library with High Confident PTM Site Localization for Phosphoproteome DIA Analysis;** Wei Zhang¹; Yue Zhou¹; Jing Li¹; ¹Thermo Fisher Scientific (China), Shanghai, China
- MP 065 **Triple Quad Two-Dimensional Scanning: A Novel Scan Approach to Highlight Relationships and Couplings between Unknowns in Complex Mixtures;** Cassandra L. Smith¹; Vincent S. Pagnotti²; ¹PPG Industries, Allison Park, PA; ²PPG Industries, Allison Park, PA
- MP 066 **A Case for Generating Organized and Comprehensive Digital Chromatogram Archives of Every Peptide Quantified in Large-Scale DIA Proteomics;** Michael R Heaven¹; Archie L Cobbs¹; Harsha P Gunawardena²; Adam J Funk³; Michael J Ford⁴; Scott A Shaffer⁵; Jeremy L Norris⁶; ¹Vulcan Analytical, Birmingham, USA; ²University of North Carolina, Chapel Hill, NC; ³University of Cincinnati, Cincinnati, Ohio; ⁴MS Bioworks, LLC Ann Arbor, MI; ⁵University of Massachusetts Medical School, Worcester, MA; ⁶Vanderbilt University, Nashville, TN
- MP 067 **Unraveling the Proteome of Differentiating Human Embryonic Stem Cells Using HDMSE/DIA MS;** Elisabeth Govaert¹; Katrien Van Steendam¹; Maarten Dhaenens¹; Liesbeth Vossaert¹; Dieter Deforce¹; ¹Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium
- MP 068 **Analysis of Phosphorylation Site and Occupancy Using Data Independent Acquisition with Electron Transfer Dissociation Mass Spectrometry;** Chein-Hung Chen¹; Ya-Ping Lin²; Chia-Lin Wu²; Jung-Lee Lin²; Chung-Hsuan Chen²; ¹Academia Sinica, Taipei, Taiwan; ²Genomics Research Center, Academia Sinica Taipei, Taiwan
- MP 069 **Using 2-Dimensional Mass Spectrometry (2DMS) for Proteomics;** Peter B. O'Connor¹; Maria van Agthoven²; Pui Yiu Lam²; Federico Floris³; Alice Lynch³; Marc-André Delsuc⁴; ¹University of Warwick, Coventry, West Midlands; ²University of Warwick, Coventry, UK; ³University of Warwick, Coventry, UK; ⁴University of Strasbourg, Strasbourg, France
- MP 070 **Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA;** Andreas Huhmer¹; Ignacio Ortea²; Michael Blank¹; Daniel Lopez-Ferrer¹; Romain Huguet¹; David Horn¹; ¹Thermo Fisher Scientific, San Jose, CA; ²IMIBIC, Cordoba, Spain

DIAGNOSTIC CLINICAL CHEMISTRY (APPLICATIONS) 071 - 094

- MP 071 **Mass Spectrometric Identification and Clarification of the in Vesica Formation of the Diuretic Chlorazanol in Sports Drug Testing Samples;** Mario Thevis¹; Hans Geyer²; Andreas Thomas²; Laura Tretzel²; Isabelle Bailloux³; Corinne Buisson³; Markus Kellmann⁴; Catharina Crone⁴; Thomas Moehring⁴; Wilhelm Schänzer²; ¹German Sport University, Cologne, NRW; ²German Sport University, Cologne, DE; ³Agence Francaise de Lutte contre le Dopage, Chatenay-Malabry, France; ⁴Thermo Fisher Scientific, Bremen, DE
- MP 072 **Development of a Sensitive and Specific LC-MS/MS Method for Rapid Diagnosis of Niemann-Pick C Disease;** Rohini Sidhu¹; Xuntian Jiang²; Sarah Gale³; David Scherrer³; Jean Schaffer³; Daniel Ory³; ¹Washington University in Saint Louis, Saint Louis, MO; ²Washington University in St. Louis, Saint Louis, MO; ³Washington University in St. Louis, St. Louis, MO
- MP 073 **A UHPLC-MS/MS Method for the Simultaneous Quantification of 10 Antihypertensive Drugs in Human Plasma;** Amedeo De Nicolò¹; Marco Simiele¹; Gabriele Bonifacio¹; Valeria Avataneo¹; Paolo Mulatero²; Franco Rabbia²; Franco Veglio²; Giovanni Di Perri¹; Antonio D'Avolio¹; ¹Laboratory of Clinical Pharmacology and Pharmacogenetic, Unit of Infectious Diseases, University of Turin, Department of Medical Sciences, Amedeo di Savoia Hospital, Turin, Italy; ²Unit of Internal Medicine, University of Turin, Department of Medical Sciences, "Città della Salute e della Scienza", Turin, Italy
- MP 074 **Multiplexed Enzymatic Assay for New-Born Screening of Mucopolysaccharidoses (type II, IIIB, IVA, VI, VII) and Neuronal Ceroid Lipofuscinosis II;** Yang Liu¹; Zdenek Spacil²; Hsuan-Chieh Liao¹; Martin Sadilek¹; Michael Gelb¹; Ronald Scott³; Frantisek Turecek¹; ¹University of Washington, Seattle, WA; ²Masaryk University, Research Centre for Toxic Compounds in the Environment, Brno, Czech Republic; ³University of Washington, Department of Pediatrics, Seattle, WA
- MP 075 **Early release of 1-pyrroline by Pseudomonas aeruginosa Cultures Discovered Using Ambient Corona Discharge Ionization Mass Spectrometry;** Juchao Liang¹; Konstantin Chingini¹; Longhua Hu²; Yaping Hang²; Huanwen Chen³; ¹East China Institute of Technology, Nanchang, China; ²The Second Affiliated Hospital of Nanchang University, Nanchang, China; ³East China University of Technology, Nanchang, Mainland
- MP 076 **Skin Transplant Quality Assessment by Multiplexed 2D MRM Mass Spectrometry – A Step Forward to Improve Clinical Success Rates;** Jingzhi Yang¹; Juncong Yang²; Andrew Percy²; Uwe vonFritschen³; Juliane C. Finke³; Christoph H. Borchers^{2,4}; Michael O. Glocker⁵; ¹Proteome Center Rostock, Rostock, Germany; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ³HELIOS Clinic Emil von Behring, Berlin, Germany; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁵Proteome Center Rostock, Rostock, Germany
- MP 077 **Quantitative Clinical Chemistry Proteomics Applied to Apolipoproteins A-I / B / C-I / C-II / C-III / E in Serum;** Yuri EM van der Burg¹; Renee Ruhaak¹; Nico PM Smit¹; Fred PHTM Romijn¹; Arnoud van der Laarse¹; Christa M Cobbaert¹; ¹Leiden University Medical Center (LUMC), Leiden, The Netherlands
- MP 078 **Characterizing Traumatic Brain Injury with New Astroglial Injury Biomarkers Measured by Targeted Mass Spectrometry;** Shen Sean¹; Julia Halford¹; Ina-Beate Wanner¹; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA



- MP 079 **High-Sensitivity, High-Throughput Quantitation of Catecholamine Metabolites in Urine by LC/MS/MS for Clinical Research;** Atsuhiko Toyama¹; Kumie Satou²; Yuki Nakamura²; Ichiro Hirano¹; ¹Shimadzu Corporation, Kyoto, Japan; ²LSI Medience Corporation, Tokyo, Japan
- MP 080 **High-Sensitivity, High-Throughput Quantitation of Catecholamines and Metanephrine in Plasma by Automated WCX-SPE Coupled to LC/MS/MS for Clinical Research;** Ichiro Hirano¹; Atsuhiko Toyama¹; Kumie Satou²; Yuki Nakamura²; Jun Watanabe¹; ¹Shimadzu Corporation, Kyoto, Japan; ²LSI Medience Corporation, Tokyo, Japan
- MP 081 **LC/MS/MS Determination of Plasma Catecholamine Metabolites Without Requiring Solid-Phase Extraction or Sample Dry-Up for Clinical Research;** Yusuke Inohana¹; Atsuhiko Toyama¹; Ichiro Hirano¹; ¹Shimadzu Corporation, Kyoto, Japan
- MP 082 **Discovery and Targeted Proteomics on Cutaneous Biopsies Infected by Borrelia for the Diagnosis of Lyme Disease.;** Benoit Westermann¹; Antoine Grillon²; Gilles Schnell¹; Benoit Jaulhac²; Nathalie Boulanger²; Laurence Ehret-Sabatier¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), CNRS-Université de Strasbourg, Strasbourg, France; ²EA7290, Virulence bactérienne précoce, groupe Borréliose de Lyme, facultés de médecine et de pharmacie, Université de Strasbourg, Strasbourg, France
- MP 083 **Increased Levels of Serum Protein Complexes are Associated with Type 2 Diabetes;** Yujie Liu¹; Bingchao Chen²; Yanmin Wang²; Mo Zhang¹; Zhili Li³; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; ²Heze Municipal Hospital, Heze, CN; ³IBMS, CAMS&PUMC, Beijing
- MP 084 **A Quantitative Assay for Serum Albumin and Creatinine in Urine Based on MALDI-TOF MS;** Stephen J. Hattan¹; Marvin Vestal²; Kenneth C Parker²; Mark Duncan^{3,4}; Jane Yang⁵; David Herold⁶; ¹Virgin Instruments/ SIMULTOF, Marlborough, MA; ²Virgin Instruments/ SIMULTOF, Marlborough, MA; ³University of Colorado, Boulder, Colorado; ⁴University of Colorado School of Medicine, Aurora, CO; ⁵University of California San Diego, La Jolla, CA; ⁶University of California, San Diego La Jolla, CA
- MP 085 **Microorganism Identification/Classification by High Resolution Tandem Mass Spectrometry with Accurate Statistical Significance;** Gelio Alves¹; Guanghui Wang²; Aleksey Ogurtsov¹; Steven Drake³; Marjan Gucek²; Anthony Suffredini³; David Sacks⁴; YI-KUO YU¹; ¹National Center for Biotechnology Information, NLM, NIH, Bethesda, MD; ²Proteomics Core, NHLBI, NIH, Bethesda, MD; ³Critical Care Medicine Department, Clinical Center, NIH, Bethesda, MD; ⁴Department of Laboratory Medicine, Clinical Center, NIH, Bethesda, MD
- MP 086 **Urinalysis of Opiates Using a Small Benchtop Instrument Combining Microfluidic Capillary Electrophoresis-ESI with High Pressure Mass Spectrometry;** Michael P Goodwin¹; Scott Mellors¹; Christopher D Brown¹; ¹908 Devices Inc., Boston, MA
- MP 087 **Rapid, Simultaneous Analysis of Urinary Monoamine Neurotransmitters and their Metabolites by UPLC-MS/MS;** Zhengzhi Xie¹; Sanjay Srivastava¹; Pawel Lorkiewicz¹; ¹University of Louisville, Louisville, KY
- MP 088 **Screening and Quantitation of Pain and Antidepressant Drugs in Human Urine by Liquid Chromatography-High Resolution Mass Spectrometry;** Ana Celia Grenier¹; Lawrence Joseph Andrade¹; ¹Dominion Diagnostics, North Kingstown, RI
- MP 089 **LC-MS Method for Quantitation of HbA1c in the Presence of the Most Common Hemoglobin Variants (S, C, D, and E);** Shawn Connolly¹; Kuanysh Kabytaev¹; Curt Rohlfing¹; Randie Little¹; ¹Department of Pathology & Anatomical Sciences University of Missouri Columbia, Columbia, MO
- MP 090 **Development of a High-Throughput Hemoglobinopathies Workflow Using High Resolution Accurate Mass Analysis;** Scott Peterman; Thermo Fisher Scientific, Grimes, IA
- MP 091 **Functionalized Surfaces for Direct Immuno-Affinity Mass Spectrometry - Detection of Haptoglobin Phenotypes;** Petr Pompach^{1,2,3}; Jana Novakova¹; Daniel Kavan^{1,2}; Oldrich Benada¹; Viktor Ruzicka⁴; Michael Volny³; Petr Novak^{1,2,3}; ¹Institute of Microbiology, Prague, Czech Republic; ²Faculty of Science, Charles University in Prague, Prague, Czech Republic; ³Affipro, Martin, Czech Republic; ⁴BioVendor, Brno, Czech Republic
- MP 092 **Identifying Vitamin D2 and D3, Their 25-OH Metabolites, and C3 Epimers in a Single LCMS Run;** Ken Tsenq¹; Toshi Ono²; Tsunehisa Hirose³; ¹Nacalai USA Inc., San Diego, CA; ²Nacalai USA Inc., San Diego, CA - California; ³Nacalai Tesque Inc., Kyoto, Japan
- MP 093 **A Simple and Effective LC/MS/MS Method Development for the Determination of Underivatized Vitamin B1 and B6 in Human Whole Blood;** Xianrong (Jenny) Wei¹; Sean Orlovicz²; ¹Phenomenex, Torrance, ca; ²Phenomenex, Torrance, CA
- MP 094 **Speciation of Fatty Acids in Human Serum by Gas Chromatography/Mass Spectrometry;** Bruce A. Benner¹; Benjamin J Place¹; Jacolin A Murray¹; ¹NIST, Gaithersburg, MD
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- MP 095 **Insights on Microsampling Implementation in Drug Discovery: Sample Collection, Matrix Effect, Recovery, Aging and Automation's Assessment for an Emerging Technology;** Graziella Bovi¹; Silvana Olivieri¹; Giuseppe Santo¹; Mariangela Corradini¹; James Rudge²; Fabio Garofolo¹; Serena Tongiani¹; ¹Angelini Research Center, Pomezia (Rome), Italy; ²Neoteryx, Torrance, CA
- MP 096 **A New Microsampling Hematocrit-Compatible Dried Plasma Card for Fully Automated Online DBSA-SPE-LC-MS/MS Bioanalysis of Opioids in Blood;** Imelda Ryona¹; Jack Henion¹; ¹Q2 Solutions, Ithaca, NY
- MP 097 **Bioanalysis of Emixustat (ACU-4429) in Whole Blood Collected with Volumetric Absorptive Microsampling by LC-MS/MS;** Zhixin Miao¹; James G Farnham¹; Glenn Hanson¹; Terry Podoll²; Michael J. Reid²; ¹Covance, Madison, WI; ²Acucela, Bothell, WA
- MP 098 **Improving Transplant Patient's Welfare; Standardising and Advancing the Therapeutic Drug Monitoring of the Immunosuppressant Drug Tacrolimus;** Dima AlMekdad^{1,2}; Mark Christian Parkin³; Chris Mussell²; ¹King's College London, London, UK; ²LGC, Teddington, UK; ³King's College London, London, United Kingdom
- MP 099 **Development and Validation of an UHPLC-MS/MS Method to Quantify Imatinib, Desmethylinatinib, Dasatinib, Nilotinib and Ponatinib in Dried Plasma Spots;** Alessandra Ariaudo¹; Simiele Marco¹; Fabio Favata¹; Luca Paglietti¹; Silvia De Francia²; Giovanni Di Perri¹; Antonio D'Avolio¹; ¹Laboratory of Clinical Pharmacology and Pharmacogenetics, Department of Medical Sciences, University of Turin, Amedeo di Savoia Hospital, Turin, Italy, Torino, Italy; ²Laboratory of Clinical Pharmacology, Department of Clinical and Biological Sciences, University of Turin, San Luigi Hospital, Orbassano (Turin), Italy, Orbassano, Italy
- MP 100 **Evaluation of Blood Fractionation Membranes for the Analysis of Dried Plasma Spots from Whole Blood Using Paper Spray Mass Spectrometry;** Brandon Bills¹; Nicholas E Manicke¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN



- MP 101 **Method Development Considerations for Paper-Spray Mass Spectrometry - Direct Ionization Technique for Physiological Fluid Analysis**; Maria C. Prieto CONAWAY¹; Jeff Patrick²; Joseph Kennedy²; Kristine Van Natta³; Marta Kozak³; ¹Thermo Fisher Scientific, San Jose, CA; ²Prosolia, Inc. Indianapolis, IN; ³Thermo Fisher Scientific, San Jose, CA
- MP 102 **Ambient Mass Spectrometric Analysis of Herbal Medicines with Flowing Atmospheric-Pressure Afterglow**; Xinyue Liang¹; Xiaoxia Gong¹; Songyue Shi¹; Mohammad Choudhury¹; Gerardo Gamez¹; ¹Texas Tech University, Lubbock, TX
- MP 103 **Evaluation of Protein Stability in Dried Plasma Spots Using Targeted and Untargeted Mass Spectrometry Techniques**; Victoria David¹; Kristine Tsantilas¹; Matthew Rosenow¹; Marissa Saltzman¹; Lizzi Neylon²; David Carpentieri²; Konstantinos Petritis²; Patrick Pirrotte¹; ¹Translational Genomics Research Institute, Phoenix, AZ; ²Phoenix Children's Hospital, Phoenix, AZ
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- MP 105 **Unsupervised Chemical Structure Assignment Based on SA-TIMS-FTICR MS Mass and Mobility Measurements for Oxygenation Products of Hydrocarbons in the Ocean**; Rebecca Marin¹; Paolo Benigni¹; Francisco Fernandez-Lima¹; Christopher Thompson²; Mark E Ridgeway²; Melvin Park²; ¹Florida International University, Miami, FL; ²Bruker Daltonic, Billerica, MA
- MP 106 **Ionization of Paraffin Samples With/Without Solvents and Analysis Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Izaak Tyson-Hirst¹; Mark P. Barrow¹; ¹University of Warwick, Coventry, United Kingdom
- MP 107 **Structural Elucidation of N-Containing Compounds in Crude Oil Using Positive Ion ESI FT-ICR MS/MS**; Ammar Nasif¹; Christianne Wicking²; Mike Hodges³; John Couves³; Huang Zeng⁴; John G Langley¹; ¹Chemistry, University of Southampton, Southampton, UK; ²BP Pangbourne Technology Centre, Pangbourne, UK; ³BP Sunbury ICBT, Sunbury, UK; ⁴BP Houston, Houston, TX
- MP 108 **Asphaltenes Generated from Low-temperature Cracking of Type II Kerogen: Molecular Characterization by Negative ESI-FT-ICR-MS and Kinetic Parameters**; Albert Kamga¹; Patrick G Hatcher²; Françoise Behar³; Francois Baudin⁴; ¹ODU Research Foundation, Norfolk, VA; ²Old Dominion University, Norfolk, VA; ³TOTAL Refining and Chemicals, Gonfreville l'Orcher, France; ⁴Universite Paris Descartes, Sorbonne Paris Cite Paris, France
- MP 109 **Structural Determination of Nitrogen-Containing Compounds in Petroleum Using Collision Cross Section Calculations (CCS) and Collision-Induced Dissociation (CID)**; Hossein Maleki¹; Sadegh Faramarzi Ganjabadi¹; Samaneh Ghassabi Kondalaji¹; Stephen James Valentine¹; ¹West Virginia University, Morgantown, WV
- MP 110 **Petroleomic Analysis of Tyre Pyrolysis Oils by Using High-Resolution ESI/APPI FT-ICR Mass Spectrometry**; Janne Janis; University of Eastern Finland, Joensuu, NA
- MP 111 **Two-Dimensional Matrix Plots for Mapping Genealogical Links in Complex Mixtures of Lignin Degradation Products**; Yulin Qi¹; Dietrich A Volmer²; ¹Saarland University, Saarbrücken, Saarland; ²Saarland University, Saarbrücken, Germany
- MP 112 **Adaptation of SARA Fractionation with Emphasis on Resins and Asphaltenes Characterization in Crude Oils with Different API Gravity Using FT-ICRMS**; Jandyson M Santos^{1,2}; Alberto Wisniewski Jr³; Marcos N Eberlin¹; Wolfgang Schrader²; ¹University of Campinas, Campinas, Brazil; ²Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany; ³Federal University of Sergipe, São Cristóvão, SE
- MP 113 **Extrography and Column Chromatography Fractionation as Tools for Increasing Compositional Space Accessibility in HRMS Analysis of Crude Oils**; Deisy Giraldo-Davila¹; Martha L. Chacon²; Marianny Y Combariza¹; Cristian Blanco-Tirado¹; Andrea Gomez-Escudero³; Jorge A Orrego-Ruiz³; ¹Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; ²Universidad Industrial de Santander, Bucaramanga, Santander; ³Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia
- MP 114 **HRMS Analysis of Naphthenic Acids Isolated from Heavy Crude Oils Using Ion Exchange and Solid Phase Extractions**; Jeferson A. Valencia-Dávila¹; Martha L. Chacón-Patiño¹; Jorge A. Orrego-Ruiz²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; ²Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia
- MP 115 **New Approaches in Petroleomics: Extending the Characterization of Nitrogen in Vacuum Residue via SPE Fractionation and Analysis by ESI FT-ICR MS**; Gessica Vasconcelos¹; Veronica Vale Carvalho¹; Carla Santos Freitas¹; Lilian Valadares Tose²; Wanderson Romão²; Rosana Cardoso Pereira³; Boniek Gontijo Vaz¹; ¹Federal University of Goiás, Goiânia, GO; ²Federal University of Espirito Santo, Vitória, Brazil; ³Petrobras, Rio de Janeiro, RJ
- MP 116 **Nitrogen Speciation in Petroleum Distillates Fractionated by SPE Using a Complementary and Powerful Approach by GC×GC-NCD and FT-ICR/MS**; Florian Albrieux¹; Ludovic Chahen²; Lyes Assam²; Fabien Chainet²; Vincent Souchon²; ¹IFPEN, Solaize, 69360; ²IFPEN, Solaize, France
- MP 117 **Asphaltene Adsorption, Aggregation and Occlusion from a High-Resolution Mass Spectrometry Point of View**; Martha Liliana Chacon-Patiño^{1,2}; Marianny Yajaira Combariza¹; Cristian Blanco-Tirado¹; Andrea Gómez-Escudero²; Jorge A Orrego-Ruiz²; ¹Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; ²Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia
- MP 118 **Petroleum Aromatic Compounds by APPI, FI, and GCEI; a Sensitivity Study**; Michael T. Cheng¹; Matthew Hurt¹; ¹Chevron Research, Richmond, CA
- MP 119 **Coupling of APPI / CS2 with Collisionally Activated Dissociation of Model Compounds for Structural Determination of Asphaltenes in Crude Oil**; Mark Romanczyk¹; Xueming Dong¹; Hilikka Kenttämää²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN
- MP 120 **High-field FT Orbitrap MS as a Competitive Alternative for the Analysis of Complex Mixtures**; Alessandro Vetere¹; Wolfgang Schrader¹; ¹Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany



- MP 121 **High-Field FT Orbitrap Mass Spectrometric Investigation on Photooxidation Processes of Crude Oil**; Ruoji Luo¹; Wolfgang Schrader¹; ¹Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany
- MP 122 **Kendrick Mass Defect Visualization of Asphaltenes Pre- and Post-Reaction with Bromine**; Michael Spiegel¹; Ian Anthony¹; Matthew Brantley¹; Alton Hassell¹; Claire Moffett¹; Subin Yoon¹; Marie Stephensen¹; Patrick Farmer¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
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- MP 124 **Detection of Picogram or Sub-Picogram Semi-Volatile Compounds by Full Scan GCMS Using a High Efficiency Source – A Game Changer?**; Dale Walker¹; Harry Prest²; ¹Agilent Technologies, Little Falls, DE; ²Agilent Technologies, Santa Clara, CA
- MP 125 **Lewisite and VX Degradation By-Product Method Development for Environmental Remediation by Liquid Chromatography/Tandem Mass Spectrometry**; Stuart Willison¹; Carolyn Koester²; Deon Anex²; Romy Campisano³; Terry O'Neill⁴; Sandip Chattopadhyay⁵; Matthew Magnuson³; ¹EPA/NHSRC, Cincinnati, OH; ²Lawrence Livermore National Laboratory, Livermore, CA - California; ³U.S. Environmental Protection Agency, Cincinnati, Ohio; ⁴MRIGlobal, Kansas City, Missouri; ⁵Tetra Tech, Cincinnati, OH
- MP 126 **Atmospheric Contaminant Source Identification Using Chemometric Approaches with Mobile Membrane Introduction Mass Spectrometry (MIMS)**; Larissa C. Richards^{1,2}; Nicholas G Davey^{1,2}; Erik T Krogh^{1,2,3}; Christopher G. Gill⁴; ¹Appl. Env. Res. Labs. (AERL), Nanaimo BC, Canada; ²University of Victoria, Victoria BC, Canada; ³Vancouver Island University, Nanaimo BC, Canada; ⁴Appl. Env. Res. Labs. (AERL), Nanaimo, BC
- MP 127 **In vivo Real-time Monitoring of Aphrodisiac Pheromone Release of Small White Cabbage Butterflies (Pieris rapae)**; Yue Li¹; Robert A Mathews²; ¹The University of Maryland, College Park, MD; ²Department of Entomology, Smithsonian Institution, National Museum of Natural History, Washington, D.C
- MP 128 **Molecular Identification of Natural Organic Matter Interactions with Mercury by Ultrahigh Resolution Mass Spectrometry**; Hongmei Chen¹; Benjamin F Mann¹; Rosalie K Chu²; Nikola Tolic²; Baohua Gu¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²Environmental Molecular Sciences Laboratory, PNNL Richland, WA
- MP 129 **Quantification of 1-Hydroxypyrene in Undiluted Human Urine Samples Using Magnetic Solid-Phase Extraction Coupled with Internal Extractive Electrospray Ionization Mass Spectrometry**; Hua Zhang¹; Haiyan Lu¹; Xiaowei Fang¹; Bi-Feng Yuan²; Yu-Qi Feng²; Huanwen Chen³; ¹East China Institute of Technology, Nanchang, China; ²Key Laboratory of Analytical Chemistry for Biology and Medicine (Ministry of Education), Department of Chemistry, Wuhan University, Wuhan, China; ³East China University of Technology, Nanchang, Mainland
- MP 130 **High Throughput Detection and Identification of Chemical Excursions via GC-MS**; Parminder Kaur¹; Corey Stedwell¹; Daniel DeBord¹; ¹1st Detect Corporation, Webster, TX
- MP 131 **That's the Law : Tracking Down Trace Levels of HBCD Isomers in Recycled Polystyrene**; Claude-Paul LaFrance¹; Maxim Maheux²; ¹TransBIOTech, Levis, QC; ²TransBIOTech, Levis, Canada
- MP 132 **Quantification of Twelve Polyfluoroalkyl Chemicals in Human Urine**; Kayoko Kato¹; Janice Ma¹; Antonia M. Calafat¹; Xiaoyun Ye¹; ¹CDC, Atlanta, GA
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- MP 134 **Tandem GC/MS Analysis of sub-pg/μL Quantities of PBDEs, Including BDE-209 Using the Novel High Efficiency EI Source**; Stephan Baumann; Agilent Technologies, Inc., Alpharetta, GA
- MP 135 **Accurate Mass Analysis of Naphthenic Acids by Ammonia NCI**; Matthew Curtis¹; Stephan Baumann¹; Mark Hewitt²; Richard Frank²; Dayue Shang³; Marcus Kim¹; ¹Agilent Technologies, Santa Clara, CA; ²Environment Canada, Burlington, Canada; ³Environment Canada, North Vancouver, BC
- MP 136 **Method optimization for Rapid Analysis of Brominated Flame Retardants in Polymers: with DART-Orbitrap HRAM**; Antonella Guzzonato¹; Olaf Scheibner²; Tabi Wang Arrey³; Thomas Moehring³; Stuart Harrad⁴; ¹University of Birmingham, Bremen, Bremen, Germany; ²Thermo Fisher Scientific, Dreieich, Germany; ³Thermo Fisher Scientific, Bremen, DE; ⁴University of Birmingham, Birmingham, United Kingdom
- MP 137 **SIFT-MS: A Complete Real-Time Solution for Analysis of Ambient Air**; Daniel B Milligan¹; David Hera¹; Thomas G Hughes^{1,2}; Nic Lamont^{1,2}; Vaughan S Langford¹; Murray J McEwan^{1,3}; Thomas I McKellar¹; ¹Syft Technologies Ltd, Christchurch, New Zealand; ²University of Canterbury, Christchurch, New Zealand; ³University of Canterbury, Christchurch, Canterbury
- MP 138 **Determination of Trace Concentrations of Carboxylic Acids and Aldehydes in Wood Smoke Particulate Matter**; Jana Rousova; University of North Dakota, Grand Forks, North Dakota
- MP 139 **Chlorinated Dioxins, Furans and Biphenyls Analysis in Complex Matrices Using Automated Extraction and Reduced Solvent Volume Column Chromatography**; Rudolf Addink¹; Philip Bassignani¹; ¹Toxic Report, Watertown, MA
- MP 140 **Automated Pressurized Liquid Extraction and Sample Clean Up of River Sediment in POPs Analysis**; Sevag Pelanjan¹; Rudolf Addink¹; ¹Toxic Report, Watertown, MA
- MP 141 **Characterization of Trihalomethanes in Meat Processing Plant Effluent**; Tiffany Liden¹; Doug D. Carlton²; Kevin A Schug²; ¹University of Texas at Arlington, Arlington, TX - Texas; ²University of Texas at Arlington, Arlington, TX
- MP 142 **Method Development for the Identification of Novel Brominated Flame Retardants Using a Q Exactive HRAM Mass Spectrometer**; Aristide P Ganci¹; Tabi Wang N. Arrey²; Thomas Moehring²; Stuart Harrad¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Thermo Fisher Scientific (GmbH), Bremen, Germany
- MP 143 **Population Assessment of Perfluoroalkyl Acids (PFAAs) in the Plasma of Wild American Alligators at Kennedy Space Center, FL**; Jacqueline T Bangma¹; John A Bowden²; Jessica Reiner²; Russell H Lowers³; Matthew P Guillelte¹; Louis J Guillelte Jr. 1; ¹Medical University of South Carolina, Charleston, SC; ²NIST, Charleston, SC; ³Integrated Mission Support Service, Titusville, FL

- MP 144 **Reducing and Normalizing Matrix Effects for the Quantification of BTEX in Contaminated Soils using Ionic Liquids in HS-GC/MS;** Emmanuel Varona-Torres¹; Michelle Reyes¹; Doug D Carlton Jr.^{1,2}; Kevin A Schug^{1,2}; ¹University of Texas at Arlington, Arlington, TX; ²Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX
- MP 145 **Ultra Low-Level Detection of Perfluoroalkyl Substances (PFASs) using LC MS/MS;** Sarah Dowd¹; Lauren Mullin²; Jennifer A Burgess²; ¹Waters Corporation, Beverly, MA; ²Waters Corporation, Milford, MA
- MP 146 **Creation of Accurate Mass Library with GC/MS Quadrupole Data and Its Application to Higher Confidence Unknown Identification;** Ming Gu¹; Yongdong Wang¹; ¹Cerno Bioscience, Norwalk, CT
- MP 147 **GC-MS/MS Determination of Synthetic Musks in Human Serum;** Ivana Kosarac¹; Cariton Kubwabo¹; Guru Prasad Katuri¹; ¹Exposure and Biomonitoring Div, Health Canada, Ottawa, ON

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- MP 149 **Analysis of Halogenated Environmental Contaminants in Food Products by Plasma-Assisted Reaction Chemical Ionization (PARCI);** Paolo Lecchi¹; Yao Lu¹; Kunyu Zheng²; Peter Haferl²; Kaveh Jorabchi²; ¹DSM Nutritional Products, Columbia, MD; ²Dept of Chemistry, Georgetown University, Washington, DC
- MP 150 **UHPLC-Liquid-El-MS/MS Interface: A New Frontier of Multiclass Environmental Risk Factors Assessment in Sudden Infant Death Syndromes;** Veronica Termopoli¹; Giorgio Famiglini¹; Pierangela Palma¹; Achille Cappiello¹; ¹University of Urbino, Urbino, Italy
- MP 151 **Fast and Robust 210 Multi-Residue Pesticide Screening of Five Washed and Unwashed Non-Organic Berries by LC-MS/MS with Simple QuEChERS Preparation;** Joshua Ye¹; Frank Kero²; Craig Young²; Sharanya Reddy²; ¹Ionics Mass Spectrometry GRO, Bolton , ON; ²PerkinElmer, Shelton, CT
- MP 152 **A Highly Specific and Robust Multi-residue Analysis of Pesticides in Water Using Time of flight in All Ion Acquisition Mode.;** Padma Marwah¹; Ashok Marwah²; Sue D'antonio³; Paul Zimba¹; ¹Texas A&M University, Corpus Christi, TX; ²Self, Corpus Christi, TX; ³Agilent technologies Inc, Cedar Creek, TX
- MP 153 **Multiplexed Analysis of 215 Pesticides Using Scout-MRM;** Romain Carriere¹; Blandine Rougemont¹; Christelle Margoum²; Mathieu Le Dréau²; David Cox³; Yves J C LeBlanc³; Jerome Lemoine¹; ¹Institut des Sciences Analytiques, UMR 5280 CNRS, Université de Lyon, Villeurbanne, France; ²IRSTEA, Villeurbanne, France; ³SCIEX, Concord, ON
- MP 154 **Automated Multi Residue Pesticides Analysis Using Pressurized Liquid Extraction and Gel Permeation Chromatography;** Philip Bassignani¹; Ruud Addink¹; ¹Fluid Management Systems, Watertown, MA
- MP 155 **Target and Not-target Screening of Pesticides and Metabolites in Paddy Water;** Eleonora Mazzucco¹; Fabio Gosetti²; Bianca Bolfi²; Marcello Manfredi³; Arianna Facchi⁴; Marco Romani⁵; Simone Silvestri⁵; Elisa Robotti²; Emilio Marengo²; ¹università Del Piemonte Orientale,

Alessandria, Alessandria; ²University of Piemonte Orientale, Alessandria, IT; ³ISALIT-DISIT, University of Piemonte Orientale, Alessandria, IT; ⁴Dipartimento di Scienze Agrarie e Ambientali, Università degli Studi di Milano, Milano, IT; ⁵Ente Nazionale Risi, Pavia, IT

- MP 156 **Rapid and Easy Comparison of Quechers Sample Preparation Methods for the Analysis of Pesticide Residues In Pear Using LC-ESI-QQQ;** Victor Manuel Mondragon Olguin¹; Jose Luis Freire¹; ¹Agilent technologies Inc, Mexico, DF
- MP 157 **Comprehensive, Sensitive, and Quantitative Screening of Pesticides in Selected Swiss Headwater Catchments by an Online-SPE-LC-Orbitrap Method;** Heinz Singer¹; Rahel Comte²; Simon Mangold²; Christoph Moschet²; Christian Stamm²; Tobias Doppler²; Irene Wittmer²; ¹Eawag, Duebendorf, CH; ²Eawag, Duebendorf, Switzerland
- MP 158 **LC-MS/MS Method Development and Validation for the Quantification of LB-100 and Endothall Metabolite in Biological Matrices;** Changyu Quang¹; Jennifer L. Simko¹; William C Nethero¹; Elizabeth A Groeber¹; John S Kovach²; ¹WIL Research, Ashland, OH; ²Lixte Biotechnology Holdings, Inc., East setauket, NY
- MP 159 **Ultra-Sensitive and Rapid Assay of Neonicotinoids, Fipronil and Some Metabolites in Honey by UHPLC-MS/MS.;** Mikael Levi¹; Aurore Jaffuel¹; Stephane Moreau²; ¹shimadzu France, Noisiel, France; ²Shimadzu Europe GmbH, Duisburg, Germany
- MP 160 **Parts-per-trillion (ppt) Level High-Throughput Quantitation of Glyphosate, Aminomethylphosphonic Acid (AMPA) and Glufosinate in Water Samples by LC-MS/MS;** Javier Lopez¹; Miguel Angel Perez¹; Carsten Baessmann²; Louis Maljers³; Joe Anacleto⁴; ¹Bruker Espanola, S.A., Madrid, Spain; ²Bruker Daltonik GmbH, Bremen , -; ³Bruker, Fremont, CA; ⁴Bruker Ltd., Milton, Canada
- MP 161 **Direct Analysis of Formulated Pesticide Product Matrices by Paper Spray Mass Spectrometry;** Khang To¹; Steven L Reeber¹; Gary Glish¹; ¹University of North Carolina Chapel Hill, Chapel Hill, NC
- MP 162 **Human Biomonitoring for Pesticide Exposure and Effects on Metabolism using Convergence Chromatography-Mass Spectrometry;** Zdenek Spacil¹; Garry Codling¹; Petra Boojij¹; Jana Klanova¹; ¹Masaryk University, Brno, Czech Republic
- MP 163 **Multiresidue Determination of non-HPLC-ESI-MS-Amenable Organochlorine Pesticides with Liquid Chromatography Dielectric Barrier Discharge Ionization Mass Spectrometry (LC-DBDI-TOFMS);** José Robles-Molina¹; Felipe J Lara-Ortega¹; Bienvenida Gilbert-López²; Antonio Molina-Díaz¹; Juan F Garcia-Reyes³; Alexander Schutz⁴; Sebastian Brandt⁴; Joachim Franzke⁴; ¹University of Jaen, JAEN, ES; ²CSIC-CIAL, Madrid, ES; ³University Of Jaen, Jaen , Andalusia; ⁴Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany
- MP 164 **An Unknown Screening Approach to Analyze Micropollutants Degradation by Different Disinfection Processes;** Julia Quilitzki¹; Patricia van Baar¹; Uwe Dünnebier¹; Olaf Scheibner²; ¹Berliner Wasserbetriebe, Berlin, Germany; ²Thermo Fisher Scientific, Bremen, Germany
- MP 165 **Removal and Transformation of Persistent Emerging Contaminants via Advanced Oxidation Techniques;** Kristin Cochran¹; Jorge Casado²; Susan Richardson¹; Dionysios Dionysiou³; Daniel Schlenk⁴; Gianluca Li Puma⁵; Danilo Russo⁶; Danilo Spasiano⁶; Marianna Vaccaro⁶; Roberto Andreozzi⁶; Nuno Reis⁶; Raffaele Marotta⁶; ¹University of South Carolina, Columbia, SC; ²Universal Diagnostics SL, Seville, Spain; ³University of Cincinnati, Cincinnati, Ohio; ⁴University of California, Riverside, Riverside, CA; ⁵Loughborough University, Loughborough,

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- United Kingdom; ⁶University of Naples Federico II, Naples, Italy
- MP 166 **Quantitation and Identification of Legal and Illicit Drugs in Wastewater in the Low ng/L Range using Large-Volume Injection and LC-MS/MS**; Paul Winkler¹; Andre Schreiber²; Michael Scherer³; ¹SCIEX, Redwood City, CA; ²SCIEX, Concord, ON; ³Sciex Switzerland, Rotkreuz, Switzerland
- MP 167 **Sensitive Screen of Pharmaceuticals and Personal Care Products (PPCPs) in Water Using Agilent 6545 LC/Q-TOF High Resolution Mass Spectrometer**; Dan-Hui Dorothy Yang¹; Craig Marvin²; mark Murphy³; Yue Song⁴; Jimmy Chan⁴; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Wilmington, DE; ³EPA, Golden, CO; ⁴Agilent, Shanghai, China
- MP 168 **Non-Target Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) – Identification of Unknown Environmental Pollutants**; Andre Schreiber¹; KC Hyland²; Paul Winkler²; ¹SCIEX, Concord, ON; ²Sciex, Redwood City, CA
- MP 169 **LCMS-MS Method for Evaluation of PPCPs in Environmental Water**; Katie M Pryor¹; Jerry Byrne II¹; Rachel Lieberman¹; Jeremy Post¹; Christopher Gilles¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- MP 170 **LC-TOF-MS and GC-MS Analysis of Pharmaceuticals and Personal Care Products in Wastewaters of Eastern North Carolina**; Blake Rushing¹; Ashley Wooten¹; Marcus Shawk¹; Mustafa Selim¹; ¹East Carolina University, Greenville, NC
- MP 171 **Analysis of Potential Genotoxic Impurities (PGI) in Active Pharmaceutical Ingredients (API) by GCMS/MS**; Prashant Hase¹; Ankush Bhone²; Durvesh Sawant²; Dheeraj Dhanu²; Sanket Chiplunkar²; Ajit Datar²; Jitendra Kelkar²; Pratap Rasam²; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, Maharashtra; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 172 **Combining Commercial and Open-Source Accurate Mass MS/MS Library Information for Suspect and Non-Target Screening Workflows**; Sascha Lege¹; Thomas Glauner²; Thierry Faye³; Craig Marvin⁴; Christian Zwiener¹; ¹Eberhard Karls University Tuebingen, Tuebingen, Germany; ²Agilent Technologies Sales&Services GmbH, Waldbronn, Germany; ³Agilent Technologies, Paris, France; ⁴Agilent Technologies, Wilmington, DE
- MP 173 **Increased Throughput in the Determination of PPCPs in Water Using Optimized MS Cycle Times in a High Sensitivity UHPLC-QQQ System**; Behrooz Zekavat¹; Thomas Glauner¹; Craig Marvin²; André Santos¹; Tarun Anumol²; Jerry Zweigenbaum²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Little Falls, DE
- MP 174 **Fates of Known and Unknown Compounds from Full Scale Ozone and Activated Carbon Adsorption Process Using High Resolution MS**; Jaewon Choi¹; Wonseok Choi¹; Hyunji Jang¹; Ilhwan Choi¹; Yuns Kim¹; Charles Yang²; Dipankar Ghosh²; ¹Kwater, Daejeon, South Korea; ²Thermo Fisher Scientific, San Jose, CA
- MP 175 **Extraction of Organochlorine Pesticides with In-line Florisil Cleanup using an Acid-Base-Neutral Solid Phase Extraction System**; Phil Germansderfer¹; Ruud Addink¹; ¹Fluid Management Systems, Watertown, MA
- MP 176 **One Step Extraction, Cleanup and Concentration of Chlorinated Pesticides in Raw Coffee Beans**; Rashid Juma¹; Ruud Addink¹; ¹Fluid Management Systems, Watertown, MA
- MP 177 **Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry**; Nan Dai¹; Shengxi Guan²; Jeremy Foster²; Ivan R. Corrêa²; ¹New England Biolabs, Ipswich, MA; ²New England Biolabs, Ipswich, MA
- MP 178 **Quantitative Histone Mass Spectrometry Identifies Elevated Histone H3 Lysine 27 Trimethylation in Melanoma**; Lauren Davis¹; Deepanwita Sengupta¹; Stephanie Byrum¹; Nathan Avaritt¹; Bradley Shields¹; Fade Mahmoud²; Matthew Reynolds¹; Lisa Orr¹; Samuel Mackintosh¹; Sara Shalin³; Alan Tackett¹; ¹Department of Biochemistry and Molecular Biology, University of Arkansas for Medical Science, Little Rock, AR; ²Department of Hematology Oncology and Internal Medicine, University of Arkansas for Medical Sciences, Little Rock, AR; ³Department of Pathology, University of Arkansas for Medical Sciences, Little Rock, AR
- MP 179 **Mass Spectrometric Profiling of Histone Proteins and Their Modifications in the Biofuel-Producing Microalgae Chlamydomonas Reinhardtii**; Carlo K Eikani¹; Aliyya Khan¹; Anthony T Iavarone²; James J Pesavento¹; ¹Department of Biology, Saint Mary's College of California, Moraga, CA; ²QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, Berkeley, CA
- MP 180 **Characterization of Histone H4 Post-translational Modification in the Microalgae Chlamydomonas Reinhardtii by Top Down Mass Spectrometry**; Aliyya Khan¹; Carlo K Eikani¹; Anthony T Iavarone²; James J Pesavento¹; ¹Department of Biology, Saint Mary's College of California, Moraga, CA - California; ²QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, CA
- MP 181 **Systems Level Analysis of Histone H3 Post-Translational Modifications Reveals Features of PTM Crosstalk in Chromatin Regulation**; Veit Schwämmle¹; Simone Sidoli²; Chrystian Ruminowicz¹; Xudong Wu^{3,4}; Chung-Fan Lee³; Kristian Helin³; Noerregaard Ole Jensen¹; ¹University of Southern Denmark, Odense, Denmark; ²University of Pennsylvania, Philadelphia, PA; ³University of Copenhagen, Copenhagen, Denmark; ⁴Tianjin Medical University, Tianjin, China
- MP 182 **Utilizing Mass Spectrometry-Based Targeted Quantitative Proteomics to Determine the Factors that Alter the Specificity of Lysine Acetyltransferases**; Yin-Ming Kuo¹; Ryan A Henry¹; Andrew J Andrews¹; ¹Fox Chase Cancer Center, Philadelphia, PA
- MP 183 **Understanding the Origin and Evolution of the Epigenetic Code of Histones with an Orbitrap Fusion Lumos**; Arnau Sebé-Pedrós¹; Cristina Chiva^{2,3}; Bernat Serra-Vidal^{2,3}; Iñaki Ruiz-Trillo⁴; Eduard Sabidó^{2,3}; ¹Weizmann Institute of Science, Rehovot, Israel; ²Proteomics Unit, Centre de Regulació Genòmica (CRG), Barcelona, SPAIN; ³Proteomics Unit, Universitat Pompeu Fabra (UPF), Barcelona, Spain; ⁴Institut de Biologia Evolutiva, Universitat Pompeu Fabra-CSIC, Barcelona, Spain
- MP 184 **Proteolytic Processing of Histone H2A by the Cathepsin L Protease**; Mariel Coradin¹; Benjamin A Garcia²; ¹University of Pennsylvania, Philadelphia, U.S.; ²University of Pennsylvania, Philadelphia, PA
- MP 185 **Introducing Epigenomics in Systems Biology: Cross-Talk between Cell Signal Transduction and Epigenetic Mechanisms**; Simone Sidoli¹; Pau Pascual Garcia¹; Katarzyna Kulej^{1,2}; Brian Debo¹; Maya Capelson¹; Benjamin A. Garcia¹; ¹Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; ²The Children's Hospital of Philadelphia, Philadelphia, PA

- MP 186 **Turnover Profiles of Histone Post-Translational Modifications in a Myogenic Model Using SILAC Labeling, Enzyme Networks and Trend Clustering Analysis;** Natarajan Bhanu¹; Simone Sidoli¹; Benjamin A Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- MP 187 **Middle-Down Characterization of Histone H4 Combinatorial Post-Translational Modification Codes for Breast Cancer Invasion;** Tingting Jiang¹; Yu Chen²; Michael E Hoover³; Christopher L Hendrickson^{1,4}; Michael A Freitas³; Alan G Marshall^{1,4}; Nicolas L Young⁵; ¹Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; ²The Roy J. Carver Biotechnology Center University of Illinois at Urbana-Champaign, Urbana, IL; ³Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH; ⁴Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; ⁵Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX
- MP 188 **LC-MS/MS for the Sensitive Quantification of 5-Methylcytidine in RNA;** Gwendolyn Gonzalez¹; Lijuan Fu¹; Yinsheng Wang¹; ¹University of California - Riverside, Riverside, CA - California
- MP 189 **Less is More: Single-Neuron Epitranscriptomics using a Tandem Mass Spectrometric Approach;** Maria Basanta-Sanchez¹; Andrea B. Kohn²; Lenka Halamkova³; Igor K. Lednev⁵; Leonid L. Moroz^{2,6}; ¹The RNA Institute, University at Albany, Albany, NY; ²The Whitney Laboratory for Marine Bioscience, St. Augustine, FL; ³The RNA Institute, University at Albany Albany, NY; ⁴The RNA Institute, Albany, NY; ⁵The RNA Institute University at Albany, Albany, NY; ⁶Department of Neuroscience and McKnight Brain Institute, University of Florida, Gainesville, FL
- MP 190 **Contributions of Quantitative Histone PTM Analysis to Target Discovery, Compound Triage, and *in vivo* Experiments into Epigenetic Drug Tolerance;** Tommy K. Cheung¹; Tobias Maile¹; Erin McNamara¹; Feng Zhao²; Patrick Trojer²; Lesley Murray¹; Marie Classon¹; David Arnott¹; ¹Genentech Inc, South San Francisco, CA; ²Constellation Pharmaceuticals, Cambridge, MA
- MP 191 **Quantitation of Post-Translational Modifications in the Nucleus: Effects of Histone Modifying Enzymes on their Histone and Non-Histone Substrates;** Anastasia Lindahl¹; Michael Smallegan²; Josue Baeza³; James Dowell²; Kimberly A Krautkramer²; John M Denu²; ¹UW-Madison, Madison; ²University of Wisconsin Madison, Madison, Wisconsin; ³Univ of Wisconsin, Madison, WI
- MP 192 ***in vitro* Characterization of Histone Acyl-Posttranslational Modifications Using LC-MS;** Johayra Simithy¹; Simone Sidoli¹; Zuo-Fei Yuan¹; Benjamin A Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- MP 193 **Probing the UV-Induced Effects on RNA and RNA-Modifications by LC-MS;** Congliang Sun¹; Zalfa Abdel-Malek¹; Kazumasa Wakamatsu²; Limbach A Patrick¹; Balasubrahmanyam Addepalli¹; ¹University of Cincinnati, Cincinnati, Ohio; ²Department of Chemistry, Fujita Health University School of Health Sciences, Toyoake, Japan
- MP 194 **Parallel Reaction Monitoring Mass Spectrometry for Histone H3 Modification Analysis of Differentiating MEL cells;** Michael Sweredoski¹; Annie Moradian¹; Matthias Raedle²; Sonja Hess³; ¹California Institute of Technology, Pasadena, CA; ²Hochschule Weihenstephan-Triesdorf, Weihenstephan-Triesdorf, Germany; ³Caltech, Pasadena, CA
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- MP 195 **HRAM LC/MS Screen for Prostaglandins found in Consumer Products;** Bethany Hanson¹; Toomey Valerie¹; ¹FDA/Forensic Chemistry Center, Cincinnati, OH
- MP 196 **Quantitation of Potential Genotoxic Impurities in Active Pharmaceutical Ingredients, Drug Products, and Process Intermediates by High Resolution LC-MS;** Robert Menger¹; James Winter¹; Alwyn Forbes¹; Andy Lo¹; Peng Wang¹; Shannon Higgins-Gruber¹; Ed Bishop¹; Naijun Wu¹; ¹Celgene, Summit, NJ
- MP 197 **Determination of Chemical Components of KABA Meteorite by LDI and ESI Ionization Methods Using a 15T FT-ICR Instrument;** Arpad Somogyi¹; Mihaly M. Nagy²; Jozsef Posta³; ¹Ohio State University, Columbus, OH; ²High School of Protestant College, Debrecen, Hungary; ³University of Debrecen, Debrecen, Hungary
- MP 198 **Origin Discrimination of Red Pepper Powder Using UHPLC-Q-Orbitrap HRMS with Multivariate Analysis;** Dong-Jin Kang¹; Ji-Young Moon¹; Seong-Hun Lee¹; ¹Experimental Research Institute, NAQS Gimcheon-si, Korea
- MP 199 **Orbitrap Fusion Tribrid Mass Spectrometer for Pharmaceutical Impurity Analysis;** Kate Comstock¹; Caroline Ding²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA
- MP 200 **MALDI spiral-TOFMS and Kendrick Mass Defect Analysis of Mycolic Acids from Bacteria which Accelerate the Formation of Antibiotics;** Kanae Teramoto¹; Shumpei Asamizu²; Taro Ozaki²; Katsuya Satoh³; Hiroyasu Onaka²; Robert Cody⁴; ¹JEOL Ltd., Akishima, Tokyo; ²The University of Tokyo, Bunkyo, Tokyo, Japan; ³Japan Atomic Energy Agency, Takasaki, Japan; ⁴JEOL USA Inc., Peabody, MA
- MP 201 **Top-down analysis of Calmodulin and Lysozyme Using MS/2DMS on an FT-ICR MS;** Federico Floris¹; Maria van Agthoven¹; Lionel Chiron²; Mark P Barrow¹; Marc-André Delsuc^{2,3}; Peter B O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²C4SC4DE, Illkirch-Graffenstaden, France; ³IGBMC, Illkirch-Graffenstaden, France
- MP 202 **Characterization of Impurities of HIV NNRTI Doravirine by High Resolution UPLC-MS and Tandem MS Analysis;** Li-Kang Zhang; Merck Research Laboratories, Kenilworth, NJ
- MP 203 **Prospecting for Aqueous Gold Clusters [37.6-kDa Au144(pMBA)60, 26.8-kDa Au102(pMBA)44] using a High-Resolution Extended-Mass-Range(EMR) Orbitrap MS;** Marcos Alvarez¹; German Plascencia-Villa¹; Wendell P. Griffith¹; David M. Black¹; Miguel José Yacamán¹; Jenny Chen²; Robert Loyd Whetten¹; ¹University of Texas at San Antonio, San Antonio, TX; ²Thermo Fisher Scientific, San Jose, CA
- MP 204 **Increased Identification of Extractables and Leachables Compounds by the Use of Chemical Ionization and Custom Databases;** Syed Salman Lateef¹; Siji Joseph¹; Ravindra Gudihal¹; ¹Agilent Technologies India Pvt. Ltd, Bangalore, India
- MP 205 **Molecular Depth Profiling with a New Hybrid 3D SIMS Instrument for Improved Molecular Identification;** Alexander Pirk¹; Rudolf Moellers¹; Henrik Arlinghaus¹; Ewald Niehuis¹; Alexander Makarov²; Stevan Horning²; Rasmus Havelund³; Melissa Passarelli³; Alex Shard³; Ian Gilmore³; ¹ION-TOF GmbH, Muenster; ²Thermo Fisher Scientific, Bremen, Germany; ³National Physical Laboratory, Teddington, United Kingdom
- MP 206 **LC-Quadrupole/Orbitrap MS/HRMS Enables Stable Isotope Resolved Simultaneous Quantification and Metabolic Isotope Tracing of Acyl-Coenzyme A Species;**



- Nathaniel W Snyder¹; Alexander J Frey¹; Sophie Trefely¹; Daniel R Feldman¹; Andrew J Worth²; Basu S Sankha³; ¹Drexel University, Philadelphia, PA; ²Bristol-Myers Squibb Pharmaceutical Candidate Optimization, Wallingford, CT; ³Department of Pathology, Brigham and Women's Hospital, Harvard Medical School, Boston, MA
- MP 207 **Quantitative Evaluation of Immunosuppressant Drugs by High Resolution Accurate Mass using Selected Ion Monitoring Analysis;** Keeley Murphy¹; Jonathan L Josephs²; Maciej P Bromirski³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Bremen, DE
- MP 208 **Parallel Untargeted and Targeted Quantitative Metabolomics for Microbiome Research;** Alexey V. Melnik¹; Fernando Vargas¹; Amina Bouslimani¹; Ivan Protsyuk²; Theodore Alexandrov^{1,2,3}; Pieter C. Dorrestein^{1,4}; ¹Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, CA; ²European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; ³SCiLS GmbH, Bremen, Germany; ⁴Departments of Chemistry, Biochemistry and Pharmacology, University of California, San Diego, CA
- MP 209 **Simultaneous Determination of Phthalic Acid Esters, Organotins, Perfluorochemicals and Flame Retardants in Plastics by HPLC-LTQ/Orbitrap Mass Spectrometry;** Li Zhang¹; Xin Luo²; Zengyuan Niu²; Xiwen Ye²; Zhixu Tang²; Shuwei Xia¹; ¹Ocean University of China, Qingdao, China; ²Shandong Entry-Exit Inspection and Quarantine Bureau, Qingdao, China
- MP 210 **Acceptance Criteria for Confirmation of Identity of Chemical Residues Using Exact Mass Data;** Hiranthi Jayasuriya¹; Philip K Kijak¹; Sherri Turnipseed²; Timothy R Croley³; Jon Wong³; Bryan Gamble⁴; Hui Li¹; ¹Center for Veterinary Medicine, FDA, Laurel, MD; ²Animal Drug Research Center, Denver, Colorado; ³CFSAN, U.S. FDA College Park, MD; ⁴Forensic Chemistry Center, Cincinnati, OH
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- MP 211 **Topographical and Chemical Imaging Using a Combined Atomic Force Microscopy/Infrared Spectroscopy/Mass Spectrometry Platform;** Vilmos Kertesz¹; Tamin Tai¹; Orsolya Karacsony¹; Vera Bocharova¹; Kevin Kjoller²; Gary J Van Berkel¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²Anasys Instruments, Santa Barbara, CA
- MP 212 **Development of Nanopipettes as Probes for Scanning Electrospray Microscopy (SESM);** Elizabeth M Yuill¹; Wenqing Shi¹; John Poehlman¹; Lane A Baker¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- MP 213 **A Reflectron Microscope-Mode Imaging Mass Spectrometer Capable of Achieving High Mass Resolution;** Ang Guo¹; Michael Burt¹; Robert Burleigh¹; Steve Thompson²; Mark Brouard¹; ¹University of Oxford, UK Oxford, United Kingdom; ²Scientific Analysis Instruments, Manchester, UK
- MP 214 **Combining Scanning Ion Conductance Microscopy and Nanospray Desorption Electrospray Ionization Mass Spectrometry for Multimodal Ambient Imaging of Biological Samples;** Julia Laskin¹; Son N Nguyen¹; Venkateshkumar Prabhakaran¹; Andrey Liyu¹; Ruichuan Yin¹; ¹Pacific Northwest National Lab, Richland, WA
- MP 215 **Combining Imaging Mass Spectrometry with Infrared Spectromicroscopy Screening: A New Approach to Studying Biological Tissues;** Antoine Masson¹; Matthew J DiTucci²; Anna Susa²; Jeremy T O'Brien¹; Evan R Williams^{1,2}; Hoi-Ying holman¹; ¹Lawrence Berkeley National Lab, Berkeley, CA; ²University of California, Berkeley, CA
- MP 216 **Ambient Submicron Mass Spectrometry Imaging by Combining AFM with MS;** Jonathan Brauer¹; Jacob Berenbeim²; Mattanah de Vries²; ¹Anasys Instruments, Santa Barbara, CA; ²University of California Santa Barbara, Santa Barbara, CA
- MP 217 **Microscope Ion Imaging of Complex Surfaces Using the Pixel Imaging Mass Spectrometry Camera;** Robert J Burleigh¹; Ang Guo¹; Edward Halford¹; Michael Burt¹; Steve P Thompson²; Mark Brouard¹; ¹University of Oxford, Oxford, UK; ²Scientific Analysis Instruments, Manchester, UK
- MP 218 **Development of Laser Capture Microdissection-Liquid Vortex Capture ESI-MS (LMD-LVC/ESI-MS) for Quantitative and Sub-Micrometer Mass Spectral Surface Sampling and Imaging;** John F. Cahill¹; Vilmos Kertesz¹; Gary J Van Berkel¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- MP 219 **Liquid Extraction Surface Analysis (LESA) Combined with Nano-Liquid Chromatography (nLC) for In-Depth Analysis of Biological Surfaces;** Daniel Eikel¹; Terry Wilper²; Karen Norton²; Eric Solon³; Sara Savage²; Simon J Prosser¹; ¹Advion, Inc. Ithaca, NY; ²Sano-Genzyme, Framingham, MA; ³QPS, Newark, DE
- MP 220 **Transmission Geometry MALDI Imaging MS: Assessing Ion Generation/Collection Efficiency at Sub-micron Laser Spot Sizes;** Andre Zavalin¹; Junhai Yang¹; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN
- MP 221 **Desorption Electrosonic Spray Ionization for Ambient Mass Spectrometry Imaging;** Shuai Guo¹; Zhili Li²; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; ²IBMS, CAMS&PUMC, Beijing
- MP 222 **Improved Reproducibility in MALDI Imaging using a Scanning Laser Beam;** Dagmar Niemeyer¹; Michael Becker¹; Shannon D Cornett²; Paul J Kowalski²; Jane-Marie Kowalski²; Sören-Oliver Deininger¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonics, Inc., Billerica, MA
- MP 223 **Laser Ablation Electrospray Ionization Mass Spectrometry Imaging (LAESI-MSI) Using an Er:YAG Laser for Improved Spot Size Resolution and Tunable Ablation;** Matthew Powell¹; Trust T Razunguzwa¹; Holly Henderson¹; Heather Anderson¹; Nicholas J. Morris¹; Todd W. Ornduff¹; David W. DuBois¹; ¹Protea Biosciences, Inc. Morgantown, WV
- MP 224 **3D nanoSIMS: A Novel High-Mass Resolution Instrument for 3D Molecular Imaging with Sub-Micron Resolution;** Melissa K. Passarelli¹; Alexander Pirkel²; Rudolf Moellers²; Ewald Niehuis²; Alexander A Makarov³; Henrik Arlinghaus²; Rasmus Havelund¹; Paulina D. Rakowska¹; Alan M. Race¹; Alex Shard¹; Andy West¹; Stevan Horning³; Peter S. Marshall⁴; Morgan R. Alexander⁵; Colin Dollyer⁴; Ian Gilmore⁶; ¹National Physical Laboratory, Teddington, United Kingdom; ²ION-TOF GmbH, Muenster, Germany; ³Thermo Fisher Scientific, Bremen, DE; ⁴GlaxoSmithKline, Stevenage, UK; ⁵The University of Nottingham, Nottingham, UK; ⁶National Physical Laboratory, Teddington, Middlesex
- MP 225 **Development of a Time and Position Sensitive Ion Detector for a Stigmatic Imaging Mass Spectrometer;** Jun Aoki¹; Yosuke Kawai¹; Yowichi Fujita²; Hisanao Hazama³; Toshinobu Hondo³; Kunio Awazu³; Michisato Toyoda¹; Yasuo Arai²; ¹Osaka University, Toyonaka, Japan; ²High Energy Accelerator Research Organization, Tsukuba, Japan; ³Osaka University, Suita, Japan
- MP 226 **Three Micron Resolution MALDI-MS Imaging Without Transmission Geometry or Oversampling and Its Application to Maize Root Cross-section;** Adam Feenstra^{1,2}; Young-Jin Lee^{1,2}; ¹Ames Laboratory-US DOE, Ames, Iowa; ²Iowa State University, Ames, IA
- MP 227 **Rapid Laser Desorption Imaging MS with Submicron Spatial Resolution;** Jerome Moore¹; J Albert Schultz²; Valerie Steen²; ¹Robot Nose, Lemont, IL; ²Ionwerks, Inc. Houston, TX



- MP 228 **DESI Imaging at Varying Acquisition Rates with Real Time Imaging Display for Optimized Tissue Imaging;** Emrys Jones¹; Mark Towers¹; Bindesh Shrestha²; Philippi Hart¹; Richard Chapman¹; Emmanuelle Claude¹; ¹Waters Corporation, Wilmslow, UK; ²Waters Corporation, Beverly, Massachusetts
- MP 229 **Automated High Throughput 3D Imaging Using Desorption Electrospray Ionisation Mass Spectrometry;** Emrys A Jones^{1,2}; Lukasz Migas³; Richard Chapman²; Emmanuelle Claude²; James Langridge²; Steven D Pringle²; Zoltan Takats⁴; Mike Morris²; ¹Imperial College London, London, Greater London; ²Waters Corporation, Wilmslow, UK; ³University of Manchester, Manchester, UK; ⁴Imperial College, London, United Kingdom
- MP 230 **Maximizing Performance of Spatial Proteomics through the Fusion of Ultra-High Speed MALDI-TOF and High Mass Resolution MALDI FTICR IMS;** Jeffrey Spraggins^{1,2,3,4}; Raf Van de Plas^{2,4,5}; Jessica L Moore^{3,4}; Daniel Ryan^{3,4}; Richard M Caprioli^{2,3,4,6}; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt Dept. of Biochemistry, Nashville, TN; ³Vanderbilt Dept. of Chemistry, Nashville, TN; ⁴Vanderbilt University MSRC, Nashville, TN; ⁵Delft University of Technology, Delft, Netherlands; ⁶Vanderbilt University School of Medicine, Nashville, TN
- MP 231 **Localization and Identification of Peptides from Tissue Using High-Speed MALDI TOF/TOF Mass Spectrometry;** Michael Becker¹; Anja Resemann¹; Janine Beckmann¹; Julian Langer^{2,3}; Rainer Paape¹; Detlev Suckau¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Max-Planck-Institute for Biophysics, Frankfurt Am Main, Germany; ³Max-Planck-Institute for Brain Research, Frankfurt Am Main, Germany

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- MP 233 **Improvement of Peptides Imaging on Tissue by Supercritical Fluid Wash of Lipids for Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry;** Shoko Matsushita¹; Noritaka Masaki¹; Kohei Sato²; Takahiro Hayasaka³; Eiji Sugiyama¹; Shu-Ping Hui³; Hitoshi Chiba³; Nobuyuki Mase²; Mitsutoshi Setou¹; ¹Department of Cell Biology and Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; ²Department of Applied Chemistry and Biochemical Engineering, Faculty of Engineering, Shizuoka University, Hamamatsu, Japan; ³Health Innovation and Technology Center, Faculty of Health Sciences, Hokkaido University, Sapporo, Japan
- MP 234 **Ammonium Sulfate Improves Detection of Hydrophilic Quaternary Ammonium Compounds through Decreased Ion Suppression in Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry;** Eiji Sugiyama¹; Noritaka Masaki¹; Shoko Matsushita¹; Mitsutoshi Setou¹; ¹Hamamatsu University School of Medicine, Hamamatsu, Shizuoka
- MP 235 **Systematic Assessment of Surfactants for MALDI Imaging Mass Spectrometry;** Bijay Banstola¹; Fabrizio Donnarumma¹; Fan Cao¹; Eulalie T Grodner¹; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA
- MP 236 **High Performance Matrix Pre-coated Targets for MALDI Imaging of Lipids;** Junhai Yang¹; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN
- MP 237 **Using MALDI Depth Profiles to Understand the Effect of ESD Sample Preparation Parameters on MALDI IMS Samples;** Brian James Malys¹; Kevin G Owens²; ¹Drexel

- University, Ambler, PA; ²Drexel University, Philadelphia, PA
- MP 238 **A Combined Enzymatic Digestion and Matrix Application Approach for High Throughput MSI of FFPE Tissue;** Haddon E. Goodman¹; Erin H. Seeley¹; ¹Protea Biosciences, Morgantown, WV
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- MP 240 **Optimal Sample Preparation Method for Visualizing Global Endogenous Metabolites by Mass Spectrometry Imaging in Arabidopsis;** Tomomi Ichinose¹; Yoshinori Fujimura¹; Shuichi Nakaya²; Yuzo Yamazaki²; Junya Nakamura¹; Eisuke Hayakawa¹; Hiroyuki Wariishi¹; Daisuke Miura¹; ¹Kyushu University, Fukuoka, Japan; ²Shimadzu Corporation, Kyoto, Japan
- MP 241 **Investigation into the use of Tissue Washing Procedures and the Subsequent Outcomes for DESI-MS Imaging Analyses;** Philippa Hart¹; Mark Towers¹; Emmanuelle Claude¹; ¹Waters Corporation, Wilmslow, UK
- MP 242 **Investigation of Aging of Chemically Fixed Mammalian Cells via ToF-SIMS;** Julia Kokesch-Himmelreich¹; Daniel J Graham¹; Lara J Gamble¹; ¹University of Washington, Seattle, WA
- MP 243 **Mass Spectrometry Imaging to Better Understand the Mycoparasitic Interaction of Biocontrol Agents;** Matthias Holzlechner¹; Zoratto Samuele¹; Reitschmidt Sonja¹; Zeilinger Susanne^{1,2}; Martina Marchetti-Deschmann³; ¹Vienna University of Technology, Vienna, Austria; ²University of Innsbruck, Innsbruck, Austria; ³Vienna University of Technology, Vienna, Vienna

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- MP 245 **Finding Patterns in Mass Spectrometry Images;** Daniel Graham¹; Lara J Gamble¹; ¹University of Washington, Seattle, WA
- MP 246 **Software for Distributed MALDI Imaging Workflows;** Stefan Frehse¹; Fingal Orlando Galashan¹; Tobias Boskamp^{1,2}; Jan Hendrik Kobarg¹; Stefan Schifferl¹; Klaus Steinhorst¹; Janina Oetjen²; Carl Evertsz¹; Theodore Alexandrov^{1,3,4}; Peter Maass^{1,2}; Dennis Trede¹; ¹SCiLS GmbH, Bremen, Germany; ²University of Bremen, Bremen, Germany; ³EMBL Heidelberg, Heidelberg, Germany; ⁴University of California, San Diego La Jolla, CA
- MP 247 **Absolute Quantification and Customizable Database Integration for Molecular Identification with MSiReader;** Kenneth Garrard¹; Mark T Bokhart¹; Milad Nazari¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC
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- MP 249 **Characterization of Data-driven Image Fusion for Imaging MS: Exploring Image Modality Combinations that Maximize Predictive Performance for Distinct Biomolecular Classes;** Raf Van de Plas^{1,2}; Jeffrey Spraggins²; Nico Verbeeck¹; Junhai Yang²; Richard M Caprioli²; ¹Delft University of Technology, Delft, Netherlands; ²Vanderbilt University, Nashville, TN

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- MP 251 **Exploring Spectral Relationships and Peak Redundancy in API Mass Spectra;** Nathaniel Mahieu¹; Gary J Patti¹; ¹Washington University in St. Louis, St. Louis, MO
- MP 252 **Accurate Mass Retention Time Locked Metabolomics EI Library and Workflows for Accurate Mass GC/Q-TOF Metabolomics Data Processing;** Sofia Nieto¹; Zijuan Lai²; Mine Palazoglu²; Hong Chen¹; Aditi Koul¹; Vadim Kalmeyer¹; Oliver Fiehn²; ¹Agilent technologies Inc, Santa Clara, CA; ²UC Davis, Davis, CA
- MP 253 **Rapid MS1 Formulae to Isotope Pattern Matching Using a Novel MS1 Search Engine for Metabolomics;** Scott Walmsley^{1,2}; Hyungwon Choi³; Samantha Bokatzian¹; Richard Reisdorph¹; Nichole A Reisdorph¹; ¹Dept. of Pharmaceutical Sci., University of Colorado Denver-Anschutz, Aurora, Colorado [CO]; ²UCD Computational Biosciences Program, Aurora, Colorado [CO]; ³National University of Singapore, Singapore, Singapore
- MP 254 **Optimus + iili: Software for LC-MS Based Spatial Metabolomics in 2D, 3D, and Virtual Reality;** Ivan Protsyuk¹; Sergey Ryazanov¹; Garg Neha²; Tal Luzzatto-Knaan²; Amina Bouslimani²; Clifford Kapon²; Alexey Melnik²; Dimitri Floros²; Luca Rappez¹; Prasad Phapale¹; Pieter Dorrestein²; Theodore Alexandrov^{1,2}; ¹EMBL, Heidelberg, Germany; ²Skaggs School of Pharmacy, UC San Diego La Jolla, CA
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- MP 256 **The 1-StoP Approach to Annotation of LC-MS Metabolomics Data;** Corey D Broeckling¹; Andrea Ganna²; Mark Layer³; Brown Kevin³; Ben Sutton³; Erik Ingelsson^{4,5}; Graham Peers³; Jessica E Prenni¹; ¹Colorado State University Proteomics and Metabolomics Facility, Fort Collins, Co; ²Broad Institute of MIT and Harvard, Cambridge, MA; ³Colorado State University, Fort Collins, CO; ⁴Uppsala University, Uppsala, Sweden; ⁵Department of Medical Sciences, Molecular Epidemiology and Science for Life Laboratory, Uppsala University, Uppsala, Sweden
- MP 257 **Utilizing Advanced Multivariate Analysis Features with Automated Database Searching Algorithms to Simplify Metabolomics Study Conduct and Understanding;** Christopher Colangelo¹; Phillip Seitzer²; Rick Schneider³; ¹Primary Ion, Old Lyme, CT; ²Proteome Software, Portland, OR; ³Pfizer, Groton, CT
- MP 258 **Automatic CCS and MS/MS Library Creation and Application for Large Scale Metabolic Profiling;** Jonathan P. Williams¹; David Eatough¹; Lee A. Gethings¹; Christopher J. Hughes¹; Mark Towers¹; Leanne Nye²; Steven Lai³; Richard Tyldesley-Worster¹; Johannes PC Vissers¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, London, United Kingdom; ³Waters Corporation, Beverly, MA
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- MP 260 **A Generalizable Method for False-Discovery Rate Estimation in Mass Spectrometry-Based Lipidomics;** Grant Fujimoto¹; Jennifer E Kyle¹; Kevin Crowell¹; Richard D Smith¹; Thomas O Metz¹; Sam Payne¹; ¹Pacific Northwest National Lab, Richland, WA

- MP 261 **Assessing Metabolic Pathways Using Chemical Kinetics Theory;** Ismael Zamora¹; Guillem Plasencia²; Laura Goracci³; ¹Lead Molecular Design, S.L., Sant Cugat del Valles, Barcelona; ²Lead Molecular Design S.L., Sant Cugat de Valles, Spain; ³Perugia University, Perugia, Italy
- MP 262 **A Computational Platform for Analysis of Stable Isotope Assisted Metabolomics Data Acquired on GC-MS;** Xiaoli Wei^{1,2}; Imhoi Koo^{1,2}; Biyun Shi^{1,2}; Pawel Lorkiewicz³; ⁴; Hamid Suhail⁵; Ramandeep Rattan⁵; Shailendra Giri⁵; Xiang Zhang^{1,2,3}; ¹Department of Chemistry, University of Louisville, Louisville, KY; ²ulatory and Center for RegEnvironmental Analytical Metabolomics, University of Louisville, Louisville, KY; ³Pharmacology & Toxicology, University of Louisville, Louisville, KY; ⁴Institute of Molecular Cardiology, University of Louisville, Louisville, KY; ⁵Henry Ford Health System, Detroit, MI
- MP 263 **Analysis of Stable Isotope Assisted Metabolomics Data Acquired by High Resolution Mass Spectrometry;** Pawel Lorkiewicz¹; Xiaoli Wei¹; Joshua Salabei¹; Biyun Shi¹; Bradford Hill¹; Seongho Kim²; Craig James McClain¹; ³; Xiang Zhang¹; ¹University of Louisville, Louisville, KY; ²Wayne State University, Detroit, MI; ³Robley Rex Louisville VAMC, Louisville, KY
- MP 264 **metax: an Automatic and Comprehensive Pipeline for Processing Metabolomics Data;** Bo Wen¹; Zhenyu Guo¹; David Broadhurst²; Yanqun Fan¹; Chunwei Zeng¹; Hui Jiang¹; Xun Xu¹; Siqu Liu¹; ¹BGI-Shenzhen, Shenzhen, China; ²University of Alberta, Edmonton, Canada

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- MP 265 **A Multi-omics Visualization Platform (MVP) Plug-in for Galaxy-based Applications;** Thomas McGowan¹; James Johnson¹; Pratik Jagtap²; Getiria Onsong¹; Candace Guerrero²; Timothy Griffin^{2,3}; ¹University of Minnesota Supercomputing Institute, Minneapolis, MN; ²University of Minnesota, Minneapolis, MN; ³Center for Mass Spectrometry and Proteomics, UMN St.Paul, MN
- MP 266 **From Start to Finish: a Complete Proteogenomic Informatics Environment Implemented in the Galaxy Platform;** Getiria Onsong¹; Pratik D Jagtap²; James E Johnson³; Thomas McGowan³; Mohammad Heydarian⁴; Karen Reddy⁵; Timothy J Griffin²; ¹University of Minnesota, Minneapolis, MN; ²University of Minnesota at Twin Cities, Saint Paul, MN; ³University of Minnesota Supercomputing Institute, Minneapolis, MN; ⁴Johns Hopkins University, Baltimore, Maryland; ⁵Johns Hopkins University, Baltimore, MD
- MP 267 **A Multi-Omic Approach to Reveal the Effect of Low-Level Gamma Radiation on Rice Seeds;** Gohei Hayashi¹; J Shibato²; A Kubo³; T Imanaka³; GK Agrawal⁴; S Shioda²; M Fukumoto⁵; G Oros⁶; Randeep Rakwal⁷; Sa Deepak⁸; Gundimeda Seetaram⁹; Upendra Simha¹⁰; Padmanaban Arunkumar¹⁰; ¹Institute of Development, Aging and Cancer, Tohoku University, Sendai, Japan; ²Hoshi University, Tokyo, Japan; ³NIES, Tsukuba, Japan; ⁴RLABB, Kathmandu, Nepal; ⁵Tohoku University, Sendai, Japan; ⁶Plant Protection Institute, Budapest, Hungary; ⁷Tsukuba University, Tsukuba, Japan; ⁸Agilent Technologies, Bangalore, Bangalore; ⁹Agilent technologies, Bangalore, India; ¹⁰Agilent Technologies (India) Pvt. Ltd., Bangalore, India
- MP 268 **Global Analysis of Lipidomics, Oxylin and Metabolomics Data Sets in Paediatric Plasmodium Falciparum Malaria;** Izabella Surowiec¹; Sandra Gouveia-Figueira¹; Tomas Skotare¹; Judy Orikiiriza²; Elisabeth Lindquist³; Sven Bergström³; Johan Normark³; Johan Trygg¹; ¹Computational Life Science Cluster (CLIC), Umeå University, Umeå, Sweden; ²Infectious Diseases Institute, School of Medicine and Health Sciences, Makerere University, Kampala, Uganda; ³Department of Molecular Biology, Umeå University, Umeå, Sweden



- MP 269 **An NGS-Independent Strategy for Proteome-Wide Identification of Single Amino Acid Polymorphisms by Mass Spectrometry;** Wenqing Shui¹; Yun Xiong²; Yufeng Guo²; Weidi Xiao³; ¹Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, Tianjin; ²Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, CN; ³Nankai university, Tianjin, China
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- MP 274 **Looking for Black Sheep: Identifying Significant Proteogenomic Outliers;** Emily Kawaler¹; Kelly V Ruggles¹; David Fenyo¹; ¹Center for Health Informatics and Bioinformatics, New York University Medical School, New York, NY
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- MP 276 **Systematic Analysis of Phosphosignaling-Affecting Mutations in a Large Clinical Breast Cancer Cohort;** Karsten Krug¹; Philipp Mertins¹; Lauren Tang¹; Jana Qiao¹; Filip Mundt¹; Karl R. Clauser¹; Michael A Gillette¹; Li Ding²; Kelly V Ruggles³; David Fenyo³; Matthew Ellis⁴; D.R. Mani¹; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Washington University School of Medicine, St. Louis, MO; ³New York University, New York, NY; ⁴Baylor College of Medicine, Houston, TX
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- MP 291 **Mass Manipulation of Ions in a Cryogenic Linear Ion Trap: Simulations and Experiment;** Larry Tesler¹; Nicolas C Polfer¹; ¹University of Florida, Gainesville, Florida
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- MP 308 **The Use of Methionine Sulfoxide Reductases to Reverse Oxidized Methionine for Mass Spectrometry Applications**; Robert Cunningham¹; Kratika Singhal²; Ryan T Fellers³; Luca Fornelli³; Henrique Dos Santos Seckler³; Bhavin Patel¹; Egle Capkauskas⁴; Juozas Siurkus⁴; Philip Compton³; John C Rogers¹; Neil L Kelleher³; ¹Thermo Fisher Scientific, Rockford, IL; ²University of Illinois at Chicago, Rockford, IL; ³Northwestern University, Evanston, IL; ⁴Thermo Fisher Scientific, Vilnius, Lithuania
- MP 309 **Top-Down sequence-specific copper and zinc retention from ECD and ETD of superoxide dismutase for ALS spinal cord**; Joe Beckman¹; Yury V Vasil'ev^{2, 3}; Nathan I Lopez^{2, 3}; Valery G Voinov^{3, 4}; ¹Linus Pauling Institute, Corvallis, OR; ²e-MSion, Inc, Corvallis, Oregon; ³Oregon State University, Corvallis, OR; ⁴Linus Pauling Institute, Oregon State University Corvallis, OR
- MP 310 **Two-Dimensional Time-Resolved LC-MS Deconvolution for Intact Mass Analysis of Biological Drugs**; Peter Haberl¹; Joe Shambaugh²; David Bush²; Maurizio Bronzetti²; Cassandra Wigmore³; Arnd Brandenburg³; ¹Genedata GmbH, Munich, Germany; ²Genedata Inc, Lexington, MA; ³Genedata AG, Basel, Switzerland
- MP 311 **Development of LC/MS/MS Bioanalytical Method for Quantitative Determination of Intact Insulin Glargine and Human Insulin in Plasma**; ZHAOQI ZHAN¹; Zhe Sun²; Jie Xing¹; Edwin Zhi Wei Ting¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore, Science Park 1; ²Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd 79 Science Park Drive #02-01/08, Singapore
- MP 312 **Enabling Mass Spectrometric Analysis of Intact Proteins in Native Conditions on A Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Kai Scheffler¹; Eugen Damoc²; Aaron Bailey³; Jonathan L Josephs³; ¹Thermo Fisher Scientific, Dreieich, DE; ²Thermo Fisher Scientific, Bremen, DE; ³Thermo Fisher Scientific, San Jose, CA
- MP 313 **Is Online Detection by Native ESI MS Beneficial to Size Exclusion Chromatography?**; Cedric Bobst¹; Igor A Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA
- MP 314 **BAC-PAGE: A Novel Proteomics Workflow Using Dissolvable Polyacrylamide Gel Electrophoresis**; Nobuaki Takemori¹; Ayako Takemori¹; Piriya Wongkongkathep²; Rachel R Ogorzalek Loo²; Joseph A Loo²; ¹Ehime University, Toon, Japan; ²UCLA, Los Angeles, CA
- MP 315 **Impact of Phosphorylation on the Ionization Efficiency of Intact Proteins: A Systematic Investigation**; Zhijie Wu¹; Wenxuan Cai²; Bifan Chen¹; Ziqing Lin²; Zachery Gregorich²; Ying Ge¹; ¹Department of Chemistry, UW-Madison Madison, WI; ²University of Wisconsin Madison, Madison, WI



- MP 316 **Magnetic Resin Microreactor for Affinity-Capture Top-Down Mass Spectrometry;** DeLafield Daniel¹; Zhe Wang¹; Woodard Toni¹; Si Wu¹; ¹University of Oklahoma, Dept. of Chem & Biochem Norman, OK
- MP 317 **High Resolving Power Isoelectric Focusing for Routine and Comprehensive Proteoform Interrogations;** Michael Tran¹; John Corbett^{1,2}; Daniel A Plymire²; Casey Wing¹; Steven M Patrie^{1,2}; ¹University of Texas at Dallas, Richardson, TX; ²University of Texas Southwestern, Dallas, TX
- MP 318 **On the Reliability and Reproducibility of 2D Isoelectric Focusing and Reversed-Phase Chromatography with FTMS for Intact Label-free Proteoform Quantitation;** John Corbett^{1,2}; Michael Tran¹; Casey Wing¹; Daniel Plymire²; Steven Patrie^{1,2}; ¹University of Texas at Dallas, Richardson, TX; ²University of Texas Southwestern Medical Center, Dallas, TX
- MP 319 **Data Independent Characterization of Proteins from 2D CID Fingerprints Generated through Collision Energy Scanning;** Boris Kozlov¹; Jeff Brown¹; John Hoyes¹; ¹Waters, Wilmslow, United Kingdom

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- MP 321 **Photodissociation of Triethylphosphonium Charge Tagged Peptides;** Nick DeGraan-Weber¹; James P Reilly¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- MP 322 **Structural Determination of Peptides Containing Multiple Acceptors using Action-EET;** Lance E Talbert¹; Ryan R Julian¹; ¹University of California, Riverside, Riverside, CA
- MP 323 **Implementation and Bench-Marking of Dual-Polarity 193 nm UVPD for Bottom-Up Proteomics on the Thermo Orbitrap Fusion Tribrid Mass Spectrometer;** Sylvester Greer¹; Jennifer S Brodbelt²; ¹Univ of Texas at Austin, Austin, Texas; ²University of Texas at Austin, Austin, TX
- MP 324 **Reaction Dynamics of Small Sulfur-Containing Molecules with a Hydrated Electron in the Gas Phase;** Chi-Kit Siu¹; Wai-Kit Tang²; ¹City University of Hong Kong, Hong Kong; ²City University of Hong Kong, Hong Kong SAR, Hong Kong
- MP 325 **Kinetic Energy Release and Fragmentation Pattern of Substituted Anilines after Collision Activation;** Sarah Seulen¹; Tassilo Muskat¹; Jürgen Grotemeyer¹; ¹Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany
- MP 326 **Photodissociation Action Spectroscopy of Fluorescent Dye Molecules in the Gas Phase;** Elena Mitrofanov¹; Tassilo Muskat¹; Claus Gernert¹; Jürgen Grotemeyer¹; ¹Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany
- MP 327 **Difference of Electron Capture and Transfer Dissociation Mass Spectrometry on Zn²⁺-Polyhistidine Complexes in the Absence of Remote Protons;** Daiiki Asakawa¹; Edwin De Pauw¹; ¹AIST, Tsukuba, Ibaraki
- MP 328 **Glycan and Peptide Analysis with Iron Oxide Nanoparticle MALDI Matrices;** Joseph Mercer Wilson¹; Qiaoli Liang¹; Jennifer Sherwood¹; Thomas Macher¹; Yuping Bao¹; Carolyn J Cassidy¹; ¹University of Alabama, Tuscaloosa, AL
- MP 329 **Characterized Fragmentation of Neutral Carbohydrates Induced by Quartz-Tungsten-Halogen Light Prior to MALDI Mass Spectrometry;** Yu-Meng Ou¹; Yin-Hung Lai¹; Yi-Sheng Wang¹; ¹Genomics Research Center, Academia Sinica Taipei, Taiwan
- MP 330 **Optimizing Production of Selected Product Ions for SRM Analysis in a Quadrupole Collision Cell;** Bennett Kalafut¹; Harald Oser¹; ¹Thermo Fisher Scientific, San Jose, California
- MP 331 **Cationized Polymer Fragmentation: Energetic and Mechanistic Effects of End-group Substitution;** Jordan M. Rabus¹; Benjamin Bythell¹; ¹University of Missouri-St. Louis, St. Louis, MO
- MP 332 **The Collision of a Hypervelocity Massive Projectile with Free-Standing Graphene: Investigation of Secondary Ion Emission and Projectile Fragmentation;** Sheng Geng¹; Stanislav S Verkhoturov¹; Michael J Eller¹; Emile A Schweikert¹; ¹Texas A&M University, College Station, TX
- MP 333 **Comparison of Ion Temperatures in a Linear Trap using the Ambient Ionization Techniques: ESI, DART and APCI;** George N. Khairallah¹; Morphy Dumlao²; Richard A J O'Hair³; William A Donald²; ¹Bio21 Inst, Uni of Melbourne and Accurate Mass Scientific P/L, Melbourne, VIC; ²University of New South Wales, Sydney, Australia; ³University of Melbourne, Victoria, Australia
- MP 334 **Exploring the Combination of Helium Charge Transfer Dissociation (He-CTD) and Hydrogen Deuterium Exchange Tandem Mass Spectrometry (HDX-MS/MSn);** Gregory C. Donohoe¹; Li Pengfei¹; Glen P. Jackson¹; Stephen J Valentine¹; ¹West Virginia University, Morgantown, WV
- MP 335 **Dissociation of Gas-Phase, Triply-Charged Lanthanide and Doubly-Charged Actinide Complexes by Multiple-Stage Tandem Mass Spectrometry;** Cassandra Hanley¹; Michael Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA
- MP 336 **Chemical Derivatization to Enhance 266 nm Ultraviolet Photodissociation for Proteomics;** M. Montana Quick¹; Rachel Mehaffey¹; Lucas D. Akin¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- MP 337 **Dissociation of Gas-Phase, Doubly-Charged Uranyl-Acetone and Uranyl-Dimethyl Sulfoxide Complexes by Collisional Activation and Infrared Photodissociation;** Theodore Corcovilos¹; Cassandra Hanley¹; Evan Perez¹; Benjamin J Bythell²; Michael J. Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA; ²University of Missouri-St. Louis, St. Louis, MO
- MP 338 **General Rules of Fragmentations Evidencing Lasso Structures in CID and ETD;** Kevin Jeanne Dit Fouque¹; Helene Lavanant¹; Severine Zirah²; Julian D. Hegemann³; Marcel Zimmermann³; Mohamed A. Marahiel³; Sylvie Rebuffat²; Carlos Afonso¹; ¹Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; ²National Museum of Natural History, CNRS-MNHN UMR 7245 Paris, FRANCE; ³Philipps University Marburg, Department of Chemistry Biochemistry LOEWE Marburg, Germany
- MP 339 **A Novel Macrobicyclic Polyether with Carbon Bridgehead Atoms: Complexation with Alkali Metals;** Anupriya Anupriya¹; David V Dearden¹; ¹Brigham Young University, Provo, UT
- MP 340 **Ab Initio Prediction of Collision-Induced Dissociation Mass Spectra;** Li Li¹; Rodger Mensing²; Benjamin Janesko²; ¹University of Texas at Arlington, Arlington, TX; ²Texas Christian University, Fort Worth, TX

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- MP 342 **Analysis of Synthetic Nucleotides using Accurate Mass and Ion Mobility;** Cynthia Sanderson¹; Sushmit Maitra¹; Keith Goodman¹; ¹SCIEX, Concord ON, Canada
- MP 343 **High Resolution Ion Mobility-Mass Spectrometry for Separation of isomers in Natural Products and Complex Mixtures;** Michael Groessl¹; Sonja Klee¹; Stephan Graf¹; ¹TOFWERK, Thun, Switzerland
- MP 344 **Frequency Encoding the Mobility of Isomeric Glycans: Separations Using Drift Tube Ion Mobility and Tandem Mass Spectrometry;** Kelsey A Morrison¹; Brad K Bendiak²; Brian H Clowers¹; ¹Washington State University, Pullman, WA; ²University of Colorado, Denver - Anschutz Medical Campus, Denver, CO
- MP 345 **Rapid and High-Throughput Detection and Quantitation of Radiation Biomarkers in Human and Nonhuman Primates by Differential Mobility Spectrometry-Mass Spectrometry;** Zhidan Chen¹; Stephen L. Coy¹; Evan L. Pannkuk²; Evagelia C. Laiakis²; Adam B. Hall¹; Albert J Jr Fornace²; Paul Vouras¹; ¹Northeastern University, Boston, MA; ²Georgetown University, Washington, DC
- MP 346 **Enhancing Carbohydrate Isomer Separation with Ion Mobility Spectrometry-Mass Spectrometry;** Xueyun Zheng¹; Xing Zhang²; Nathaniel S Schocker³; Roger A Ashmus³; Igor C Almeida³; Keqi Tang¹; Catherine E Costello⁴; Richard D Smith¹; Katja Michael³; Erin Baker¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Colorado, Denver, CO; ³University of Texas, El Paso, TX; ⁴Boston University School of Medicine, Boston, MA
- MP 347 **Evaluation of Collision Cross Section Calibrants for Structural Analysis of Lipids by Traveling Wave IM-MS;** Kelly M Hines¹; Jody C May²; John A McLean²; Libin Xu¹; ¹University of Washington, Seattle, WA; ²Vanderbilt University, Nashville, TN
- MP 348 **Rapid Differentiation of Bile Acid Isomers Using Sodiated Multimer Complexes with Ion Mobility - Mass Spectrometry;** Robin H.J. Kemperman¹; Christopher D Chouinard¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL
- MP 349 **Machine Learning-Enabled Collisional Cross Section Predictor (CCSP) for Identification of Unknown Lipids;** Molly T Soper-Hopper¹; Nga Lee Ng¹; Nicholas V Hud¹; Charles Liotta¹; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta
- MP 350 **Reducing Isobaric Species by Differential Mobility Spectrometry (DMS) for infusion-based lipidomics;** Goncalo Vale¹; Jeff McDonald¹; Paul RS Baker²; ¹UT Southwestern Medical Center, Dallas, TX; ²Sciex, Framingham, MA
- MP 351 **Characterization of Exposome Compounds in Human Biofluids Using LC-ESI-Ion Mobility QTOF Mass Spectrometry;** Yunjia Lai¹; Mine Palazoglu¹; Oliver Fiehn¹; ¹UC Davis Genome Center, Davis, CA
- MP 352 **Increasing the Resolving Power of Differential Mobility to Supplement (or Eliminate) LC Separation;** J.C. Yves Leblanc¹; Chang Liu²; Larry J Campbell²; Brad Schneider²; ¹SCIEX, Concord, ON, ON; ²SCIEX, Concord ON, Canada
- MP 353 **Enhanced Ion Mobility Separation of Derivatized Isobaric Steroids by DESI and MALDI TOF Mass Spectrometry;** Mark Towers¹; MicShazia Khan²; C.Logan C Mackay³; Ruth Andrew²; Emmanuelle Claude¹; ¹Waters Corporation, Wilmslow, UK; ²Queen's Medical Research Institute, University of Edinburgh, Edinburgh, UK; ³SIRCAMS, University of Edinburgh, Edinburgh, UK
- MP 354 **Rapid separation of Vitamin D epimers in human serum by Liquid Chromatography Ion Mobility Mass Spectrometry;** Nicholas Oranzi¹; Christopher D Chouinard¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL
- MP 355 **Combining Rapid Isomer Separations and Physicochemical Property Predictions for Drug Molecules with Differential Mobility Spectrometry;** CHANG LIU¹; Yves J C LeBlanc¹; Jeffry Shields²; Hui Zhang²; John S Janiszewski²; Christian Ieritano³; Luke Melo³; Evan Shepherson³; Mitch Verbuyst³; Moaraj Hasan³; Dalia Naser³; Scott W Hopkins³; Larry J Campbell¹; Tim Hoffman¹; ¹SCIEX, Concord, ON; ²Pfizer, Groton, CT; ³University of Waterloo, Waterloo, Ontario (ON)
- MP 356 **Complicated Natural Product Analysis Using Liquid Chromatography (LC) – Drift Tube Ion Mobility (DTIM) Mass Spectrometry (MS);** Xin Ma¹; Tao Bo²; ¹Agilent Technologies, Beijing, China; ²Agilent Technologies (China) Limited, Beijing, China
- MP 357 **Structural Database of Secondary Metabolites for Natural Product Discovery: Ion Mobility-Mass Spectrometry Measurements in Nitrogen and Helium Drift Gases;** Andrzej Balinski¹; Jody C May¹; Brian O Bachmann¹; Sarah M Stow¹; John A McLean¹; ¹Vanderbilt University, Nashville, TN
- MP 358 **Determining Molecular Modifications by ESI Ion Mobility Mass Spectrometry (ESI IM-MS);** Alfred L. Yergey¹; Paul S Blank¹; Stephanie M Cologna²; Peter S Backlund¹; Allan Darling³; ¹NIH, Bethesda, MD; ²University of Illinois, Chicago, IL; ³Vtess Inc, Gaithersburg, MD
- MP 359 **Analysis of Propolis Extracts and Isomeric Flavonoid Mixtures Using Trapped Ion Mobility QTOF-MS;** Sven Wolfgang Meyer¹; Alexander Harder²; Detlev Suckau³; Peter Sander³; ¹Bruker Daltonic GmbH, Bremen, Bremen; ²Bruker Daltonic, Bremen, Germany; ³Bruker Daltonic GmbH, Bremen, Germany
- MP 360 **Investigation of the Cu(I) and Zn(II) Binding Characteristics of Methanobactin from *Methylosinus trichosporium* OB3b;** Jacob Watson McCabe¹; Rajpal Vangala¹; Laurence Ambrose Angel¹; ¹Texas A&M University - Commerce, Commerce, TX
- MP 361 **Single Oligomer Polyurethane Synthesis: Characterization by Ion Mobility-Mass Spectrometry and Computational Strategies;** Tiffany Crescentini^{1,2}; Sarah M Stow^{1,2}; Robert W. Davis^{1,2}; Gary A. Sulikowski^{1,2,3}; David M Hercules^{1,2}; John A McLean^{1,2}; ¹Vanderbilt Dept. of Chemistry, Nashville, TN; ²Vanderbilt University, Nashville, TN; ³Vanderbilt Institute of Chemical Biology, Nashville, TN
- MP 362 **Characterization of Conformational Isomers of Bisthienylethenes (BTEs) Using Ion Mobility Mass Spectrometry;** Xu Wang¹; Ming Wang¹; Alejandro Cisneros¹; Xiaopeng Li¹; ¹Texas State University, San Marcos, TX
- MP 363 **Enhancing Analytical Characterization Workflows of Complex Synthetic Polymeric and Small Molecule Mixtures through Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS);** John Patrick O'Brien¹; Jeffrey R Gilbert²; Bruce M Bell¹; ¹The Dow Chemical Company, Midland, MI; ²Dow AgroSciences, Indianapolis, IN
- MP 364 **Comparison of Ion Mobility Mass Spectrometry Applications on Commercial Drift-Tube and Differential Mobility Based Instruments;** Jeffrey Gilbert¹; Jesse L Balcer¹; John O'Brien²; David McCaskill¹; Yelena A Adelfinskaya¹; Gerrit J Deboer¹; Cassie Phaner²; Krishnamoorthy Kuppannan²; Mary D Evenson¹; Lisa Buchholz¹; Bruce Bell²; ¹Dow AgroSciences, Indianapolis, IN; ²Dow Chemical Company, Midland, MI
- MP 365 **Separation of Positional Isomers of PAHSAs Using LC-MS/MS Coupled with Differential Ion Mobility Mass Spectrometry;** Shaokun Pang¹; Liling Liu²; Xiaorong Liang²; Amos Baruch²; Leo Wang¹; Brian Dean²; Yuzhong Deng²; ¹SCIEX, Redwood City, CA; ²Genentech Inc, South San Francisco, CA

- MP 366 **Structural Dependent Section of Calibrants for Accurate Measurement of CCS Values Obtained with Ion Mobility Mass Spectrometry**; Dongwan Lim¹; Arif Ahmed¹; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, Republic of Korea
- MP 367 **Enantiomer Separation of Amino Acids through Binuclear Copper Bound Complex by Travelling Wave Ion Mobility Mass Spectrometry**; Xiang-Ying Yu¹; Zhong-Ping Yao^{1,2}; ¹State Key Laboratory of Chinese Medicine and Molecular Pharmacology (Incubation), Shenzhen Research Institute of The Hong Kong Polytechnic University, Shenzhen, China; ²Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China
- MP 368 **Maintaining Speciation of Reactive Gas-Phase Complexes for the Metals Uranyl, Barium, Cesium and Lanthanum with Sulfoxides using AP-IMS-MS**; Austen Davis¹; Brian H Clowers¹; ¹Washington State University, Pullman, WA
- MP 369 **Ion Mobility Mass Spectrometry of Polyoxometalate Anion Assemblies**; Helene Lavanant¹; Sebastien Hupin¹; Michael Groessl²; Madeleine Piot³; Guillaume Izzet³; Carlos Afonso¹; ¹Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; ²TOFWERK, Thun, Switzerland; ³Sorbonne Univ, CNRS UMR 8332 IPMC Paris, France
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- MP 371 **On-line Parallel Accumulation – Serial Fragmentation (PASEF) for Shotgun Proteomics on a Modified UHR-QTOF Platform**; Scarlet Beck¹; Florian Meier¹; Jürgen Cox¹; Markus Lubeck²; Stephanie Kaspar-Schoenefeld²; Nicole Drechsler²; Niels Goedecke²; Melvin Park³; Oliver Raether²; Matthias Mann¹; ¹Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; ²Bruker Daltonic GmbH, Bremen, Germany; ³Bruker Daltonic, Billerica, MA
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- MP 374 **Radical Cations of Nucleobases: A Gas-Phase Reactivity and Structural Elucidation Study**; Michael Lesslie¹; Lawler T John¹; Courtney Kanak¹; Ryzhov Victor¹; ¹Northern Illinois University, DeKalb, IL
- MP 375 **Gas-Phase Reactions of the Deprotonated Nucleobases with H, N, and O Atoms**; Charles Nichols¹; Zhe-Chen Wang¹; Carl W Lineberger¹; Veronica M Bierbaum¹; ¹University of Colorado, Boulder, CO
- MP 376 **Charge Transfer Dissociation (CTD) of Phosphocholines: Gas-Phase Ion/Ion Reactions between Helium Cations and Phospholipid Cations**; Pengfei Li¹; Glen P Jackson¹; ¹West Virginia University, Morgantown, WV
- MP 377 **DNA/Peptide Complex Ion Dissociations: Survivor Non-Covalent Sites in “Three-Body” Product Ions Independent on Charge Polarity**; Bessem Brahimi¹; Sandra Alves¹; Jean-claude Tabet^{1,2}; ¹University Paris VI (UPMC) case 45 UMR 8232 CNRS, Paris Cedex 05, France; ²CEA, iBiTec-S SPI LEMM Gif Sur Yvette, France
- MP 378 **Modulating the Interaction of Non-Covalent Dimers with Conformationally Restricted Peptides in the Gas Phase**; Huong (Ivy) Thi Huynh Nguyen¹; Frantisek Turecek²; ¹University of Washington, Department of Chemistry Seattle, WA; ²University of Washington, Seattle, WA
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- MP 382 **Distinguishing Hexose Isomers by Lithiated Ion Adduction to Water**; Matthew Campbell¹; Chen Dazhe²; Gary L. Glush²; ¹UNC, Chapel Hill, NC; ²UNC-Chapel Hill, Chapel Hill, NC
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- MP 385 **Dual-Electrospray Synthesis and Reactions**; Shaan Rashid¹; Paul Michael Mayer²; ¹University of Ottawa, Ottawa, Canada; ²University of Ottawa, Ottawa, ON
- MP 386 **Efficient and Direct Amide Bond Formation Using a Novel Alcohol/Amine Cross-Coupling Reaction Mediated by Electrospray-Based Photo-catalysis**; Savithra Jayaraj¹; Qiongqiong Wan¹; Abraham Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 387 **PhenylNitrenium Ions: Gas-phase Synthesis, Properties in Selective Alkane Activation, Gas-phase acidity, Hydride Affinity, Electron Affinity, and Electronic states**; Lei Yue¹; Pan Yuanjiang¹; Ding Chuanfan²; ¹Zhejiang University, Hangzhou, China; ²Fudan University, Shanghai, China

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- MP 391 **Substituent Effects on the Reactivity of the 2,6-Didehydropyridinium Cation, an Unusual meta-Benzyne**; Xin Ma¹; Joann P. Max¹; Duanda Wang¹; John J. Nash¹; Hilikka I. Kenttämää¹; ¹Department of Chemistry, Purdue University, West Lafayette, IN
- MP 392 **Differentiation of Deprotonated Dihydroxybenzene Regioisomers via Ion-Molecule Reactions with Thionyl Chloride**; Hanyu Zhu¹; Hilikka I Kenttämää¹; ¹Purdue University, West Lafayette, IN
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- MP 396 **Gas-Phase Reactivity of Isomeric σ,σ -Biradicals: A Comparison of 1,4-, 1,3-, and 3,4-Didehydroisoquinolinium Cations**; Lucas Szalwinski¹; Nelson R Vinuesa¹; John Nash¹; Hilikka Kenttämää¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN
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- MP 399 **Action-Excitation Energy Transfer Illuminates the Impact of Amino Acid Epimerization and Isomerization on Peptide Structure**; Dylan Riggs; University of California - Riverside, Riverside, CA
- MP 400 **Microsolvation by 18-Crown-6 as a Method for Preserving Native-Like Protein Structure**; James Bonner¹; Nathan Hendricks¹; Ryan R Julian¹; ¹UC Riverside, Riverside, CA - California
- MP 401 **Thermochemical Differences in Isomeric Oligopeptides: Structural Insights Using IRMPD Spectroscopy**; Patrick Henry Batoon¹; Jianhua Ren²; Jos Oomens³; Giel Berden³; ¹University of the Pacific, Stockton, CA; ²University of the Pacific, Stockton, CA; ³FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands
- MP 402 **Deep Molecular Structure Probing in MS_n by IR Ion Spectroscopy: Deamidation Reaction Networks of Gln and Asn-Containing Dipeptides**; Jos Oomens^{1,2}; Lisanne JM Kempkes¹; Jonathan Martens¹; Josipa Grzetic¹; Giel Berden¹; ¹Radboud University, Nijmegen, Netherlands; ²University of Amsterdam, Amsterdam, The Netherlands
- MP 403 **Infrared Spectroscopy of Protonated and Radical Cationic Triphenylamine**; Giel Berden¹; Md. Musleh Uddin Munshi¹; Jonathan Martens¹; Jos Oomens¹; ¹FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands
- MP 404 **The Remarkable Ionic Coordinating Ability of All-cis 1,2,3,4,5,6 Cyclohexane in the Gas Phase**; Terry McMahon¹; Blake Ziegler²; Michael Lecours²; Rick Marta²; Eric Fillion²; Scott W Hopkins³; David O'Hagan⁴; Keddie Neil⁴; ¹University of Waterloo, Waterloo, ON; ²University of Waterloo, Waterloo, ON, Canada; ³University of Waterloo, Waterloo, Ontario (ON); ⁴University of St. Andrews, St. Andrews, UK
- MP 405 **Laser Spectroscopic Investigation on Dichlorofluorobenzenes by Means of Resonance Enhanced Multiphoton Ionization and Mass Analyzed Threshold Ionization**; Sascha Krüger¹; Jürgen Grottemeyer¹; ¹Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany
- MP 406 **New Insights into the Combustion Chemistry of Butane Isomers in Premixed Low-Pressure Hydrogen Flames by Imaging Photoelectron Photoion Coincidence Spectroscopy**; Thomas Bierkandt¹; Yasin Karakaya¹; Dominik Krüger²; Patrick Hemberger³; Patrick Oßwald²; Markus Köhler²; Tina Kasper¹; ¹University of Duisburg-Essen, Duisburg, Germany; ²Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany; ³VUV Spectroscopy Group, Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland
- MP 407 **Förster Resonance Energy Transfer as a Distance Probe for Gas-phase Ubiquitin Ions**; Jocky Chun Kui Kung¹; Martin F Czar¹; Benjamin Schuler²; Rebecca A Jockusch¹; ¹University of Toronto, Toronto ON, Canada; ²University of Zurich, Zurich, Switzerland
- MP 408 **Alkali Cation Chelation in Cold β -O-4 Tetralignol Complexes**; Andrew F DeBlase¹; Eric T Dziekonski¹; John R Hopkins¹; Nicole L Burke¹; Huaming Sheng¹; Hilikka I Kenttämää¹; Scott A McLuckey¹; Timothy S Zwier¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN
- MP 409 **Development and Performance of a Mass Selective Linear Ion Trap for Infrared Predissociation Spectroscopy of Metabolites**; Adam Cismesia¹; Nicolas C Polfer¹; ¹University of Florida, Gainesville, Florida
- MP 410 **Photodissociation Dynamics in Infrared Multiple Photon Dissociation Monitored by Time-of-Flight Mass Spectrometry**; Matthew Bell¹; Nicolas C Polfer¹; ¹University of Florida, Gainesville, FL
- MP 411 **Gas Phase Fluorescence Spectroscopy for the Study of Catalytic Nitrogen-Containing Heterocycles**; Alessandra Ferzoco¹; Vaishnavi Rajagopal¹; ¹Rowland Institute at Harvard, Cambridge, MA
- LC-MS: CHROMATOGRAPHY AND SOFTWARE (PART 1)**
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- MP 412 **Demonstration of Automated On-The-Fly Retention Time Updating and SRM Method Visualization for Targeted Peptide Quantitation**; Susan Abbatiello¹; Qingyu Song²; Mary Blackburn²; Jacek W Sikora³; Paul

- Martin Thomas³; Neil Kelleher³; Yupeng Zheng³; Vane Dhevi Sanghvi²; ¹Thermo Fisher Scientific, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA; ³Kelleher Research Group, Evanston, IL
- MP 413 **An Interactive Skyline Tool for Flagging Incorrectly Chosen Peptides Peaks Across Data-Independent Acquisition Experiments: AT-Peptide Peak Picking (AT-P3);** Andy Lin¹; Jarrett D Egerton¹; Brooke Nuun¹; Michael J MacCoss¹; ¹University of Washington, Seattle, WA
- MP 414 **Column Performance: Comparison of Superficially Porous Particle (SPP) to Fully Porous Particles (FPP);** Rob Freeman¹; Sharon Lupo¹; Shun-Hsin Liang¹; Frances Carroll¹; Ty Kahler¹; Susan Steinike¹; ¹Restek Corporation, Bellefonte, PA
- MP 415 **High Resolution LC/MS analysis of Therapeutic Oligonucleotides on a New Porous Polymer-Based Reversed Phase Column;** Shanhua Lin¹; Julia Baek¹; Jim Thayer¹; Hongxia Wang²; Jonathan L Josephs²; Xiaodong Liu¹; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, San Jose, CA
- MP 416 **Slightly Bigger is Better: Nano-LCMS with 100um ID columns;** Brett Larsen¹; Joshua Sandor¹; Meghan McFadden¹; Anne-Claude Gingras^{1,2}; ¹LTRI, Toronto, Canada; ²Department of Molecular Genetics, University of Toronto, Toronto, Canada
- MP 417 **Improving Sensitivity in LC/MS with Multi-Dimensional Chromatography;** Thomas E. Wheat¹; Amanda B. Dlugasch²; Patricia R. McConville²; ¹Waters Corporation, Hopedale, MA; ²Waters, Milford, MA
- MP 418 **Maximizing Flexibility: A Gas and Temperature Enabled Chip-Based Solution for Nanoflow and Microflow LC-MS;** Helena Svobodova¹; Aaron Dewberry¹; Amanda Berg²; Gary A Valaskovic¹; ¹New Objective, Woburn, MA; ²New Objective, Inc., Woburn, MA
- MP 419 **Achieving High Proteome Coverage by Miniaturization of HPLC Columns;** Annie Moradian¹; Roxana Eggleston-Rangel¹; Michael Sweredoski¹; Sonja Hess¹; ¹California Institute of Technology, Pasadena, CA
- MP 420 **Sphingolipid Profiling Using Robust and Sensitive LC-MS-MS Method;** Shachi Saluja¹; Dhipankar Malakar²; Manoj Pillai²; Avinash Bajaj¹; Ujjaini Dasgupta³; ¹Regional Centre for Biotechnology, Faridabad, India; ²Sciex, Gurgaon, India; ³Amity University, Gurgaon, India
- MP 421 **Evaluation of Critical Column Parameters for Use in Supercritical Fluid Chromatography by SFC-MS;** Alison Wicker¹; Doug D. Carlton Jr.¹; Ty Kahler²; Kevin A Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²Restek Corporation, Bellefonte, PA
- MP 422 **Advancing Separation Sciences under Alkali Conditions Using a Novel C18 Column for LC-MS;** Itaru Yazawa¹; Yasuo Yamamori²; Hiroshi Tachikawa²; ¹Imtakt Corporation, Kyoto, Japan; ²Imtakt Corporation, Kyoto, Japan
- MP 423 **Analysis of Antioxidants in Yam (Dioscorea alata L. var. Purpurea (Roxb.) M. Pouch.) by HILIC- UV-ECD-MS;** Chih-Hsien Wang¹; Gao-Fong Chang¹; Wenlung Chen¹; Tsai-Fei Yu¹; Ya-Chi Feng¹; Kuo-Lung Ku²; ¹Department of Applied Chemistry, National Chiayi University, Chiayi City, Taiwan; ²National Chiayi University, Chiayi City, Chiayi
- MP 424 **Displacement Chromatography Applied for Two-Dimensional Liquid Chromatography Coupled to Tandem Mass Spectrometry for Analysis of Complex Biomolecule Mixtures;** Hartmut Schlüter¹; Marcel Kwiatkowski²; ¹UKE - Mass Spec Proteomics, Hamburg, Hamburg; ²UKE - Mass Spec Proteomics, Hamburg, Germany
- MP 425 **Combined New Approaches for Improved Quantitative and Qualitative LC-MS;** Stephan Altmair¹; Hans Griesinger¹; Michael Schulz¹; ¹Merck, Darmstadt, Germany
- MP 426 **Rapid Separation and Determination Of 25-Hydroxy Vitamin D2 / D3 in Serum By UHPLC-MS/MS Using A Novel C18-PFP Stationary Phase ;** Geoffrey Faden¹; Alan P McKeown²; ¹MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; ²Advanced Chromatography Technologies Ltd, Aberdeen, -
- MP 427 **Separation and Low Level Determination Of Catecholamines: Epinephrine, Norepinephrine and Dopamine from Plasma By UHPLC-MS/MS Using A Novel C18-PFP Column;** Edward Faden¹; Alan P McKeown²; ¹MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; ²Advanced Chromatography Technologies Ltd, Aberdeen, -
- MP 428 **LC/MS as a Monitoring Technique for (semi) Preparative Electrochemical Metabolite Synthesis;** Lisa Frensemeier¹; Uwe Karst¹; ¹University of Münster, Münster, DE
- MP 429 **Increased MS Protein Identification Rates Using 75 cm Long nano LC C18 Separation Columns: Pushing the Limits of Bottom-Up Proteomics;** Daniel Lopez-Ferrer¹; Michael Blank¹; Stephan Meding²; Aran Paulus¹; Romain Huguet¹; Remco Swart²; Andreas FR Huhmer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Germering, Germany
- MP 430 **Influencing the Selectivity of Small Proteins and Peptides on the Raptor™ ARC-18;** Susan Steinike¹; Shun-Hsin Liang¹; Sharon Lupo¹; Frances Carroll¹; Ty Kahler¹; ¹Restek Corporation, Bellefonte, PA
- MP 431 **Extraction and Ionization Efficiency in On-line Supercritical Fluid Extraction and Chromatography–Mass Spectrometry for Protease Inhibitors and Steroids in Blood;** Laura Akbal¹; Michel Raetz¹; Kyoko Watanabe²; Yasuhiro Funada²; Gérard Hopfgartner¹; ¹University of Geneva, Geneva, Switzerland; ²Shimadzu, Kyoto, Japan
- MP 432 **Maximizing Throughput of Shotgun Proteomics by Increasing the Internal Diameter of Nano-Capillary Columns;** Yuan-wei Nei¹; Danielle B Gutierrez¹; William J Burns²; Ashley T Jordan²; Jeremy L Norris¹; Richard M Caprioli¹; ¹Vanderbilt University MSRC, Nashville, TN; ²Vanderbilt University Medical Center, Nashville, TN
- MP 433 **Fast Chromatography For Quantitative Proteomics Workflows;** Alina Asteffani¹; Garry Corthals²; Petra Jansen¹; Michelle Camenzuli¹; Andrea Gargano¹; ¹University of Amsterdam, Amsterdam, The Netherlands; ²University of Amsterdam, Amsterdam, ZH
- MP 434 **Improved Sensitivity for Characterization of Sulfonamides and Trimethoprim in Honey Using QuEChERS Extracts with LC-MS/MS;** Hernando Escobar¹; Jeffrey H Dahl¹; Eddie Medina¹; Christopher T Gilles¹; ¹Shimadzu Scientific Instruments, Inc., Columbia, MD
- MP 435 **Quantitative Analysis of Oligonucleotides Using Liquid Chromatography Coupled with High Resolution/ Accurate Mass (HR/AM) Mass Spectrometry;** Nidhi Jaiswal¹; David M Good²; Marc Browning¹; Benjamin Johnson¹; Emily Measom¹; Cassidy Hatch¹; Min Meng¹; Scott A Reuschel¹; Troy Voelker¹; ¹Covance, Salt Lake City, UT; ²Covance, Madison, WI
- MP 436 **Complementary ERLIC and RPLC Online Separations Significantly Expand Sequence Coverage in MS-Based Proteomic and Proteogenomic Studies;** Candace Guerrero¹; Pratik D Jagtap¹; James Johnson²; Thomas F McGowan²; Tim Griffin³; ¹University of Minnesota, Minneapolis, MN; ²University of Minnesota Supercomputing Institute, Minneapolis, MN; ³University of Minnesota at Twin Cities, Saint Paul, MN
- MP 437 **A Direct Comparison between Ultrafiltration and Online Size Exclusion Affinity Selection Mass Spectrometry Methods;** Christopher Reutter¹; Manuel Molina-Martin²;



- Elizabeth Wright¹; Jibo Wang¹; Ryan Bernhardt¹; Kevin McLeaster¹; Eduardo Harguindeguy²; Miriam del Prado²; Alfonso Espada²; Juan Espinosa²; Michael J Chalmers¹; Keith Burton¹; ¹Eli Lilly and Company, Indianapolis, IN; ²Eli Lilly and Company, Alcobendas, Spain
- MP 438 **An Online 2D RP-RP LC/MRM-MS Method Provides Higher Sample Throughput for the Analysis of the Human Plasma Proteome**; Richard R Vincent¹; Andrew J Percy²; Dominik Domanski^{1,3}; Christoph H. Borchers^{1,2,4}; ¹Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC, CANADA; ³University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 439 **NanoLC-MS of Intact Histones by 0.5 µm Nonporous Silica Particles for Top-Down Proteomics**; Ximo Zhang¹; Michael E Hoover²; Luca Fornelli³; Philip Compton³; Michael A Freitas²; Neil L Kelleher³; Mary Wirth¹; ¹Purdue University, West Lafayette, IN; ²The Ohio State University, Columbus, Ohio; ³Northwestern University, Evanston, IL
- MP 440 **Autopiquer – Introducing a New Approach to High Confidence Peak Detection**; David Kilgour¹; Sam Hughes²; David J Clarke³; Quoc Bao Tran⁴; Clare Coveney¹; David J Boock¹; Logan C Mackay³; Young Ah Goo⁴; David R Goodlett⁴; ¹Nottingham Trent University, Nottingham; ²University of Edinburgh, Edinburgh, UK; ³University of Edinburgh, Edinburgh, United Kingdom; ⁴University of Maryland School of Pharmacy, Baltimore, MD
- LIPIDS: GENERAL
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- MP 441 **Selective Extraction of Phospholipids from Biological Sample with Metal Oxide Chromatography for Mass Spectrometry-Based Analysis**; Shota Miyazaki¹; Yuko Yui¹; Shigenori Ota¹; Kosuke Osaka²; Mamoru Kyogashima³; Atsushi Sato¹; ¹GL Sciences Inc., Saitama, Japan; ²GL Sciences Inc., Tokyo, Japan; ³Nihon Pharmaceutical University, Saitama, Japan
- MP 442 **Evaluation of Docosahexaenoic Acid Derived Lipid Mediators after Traumatic Brain Injury by a Global LC-MS/MS Method**; Tamil Selvan Anthonymuthu¹; Lewis Jesse¹; Andrew A Amoscato¹; Patrick M Kochanek¹; Kagan E Valerian¹; Hulya Bayir¹; ¹University of Pittsburgh, Pittsburgh, PA
- MP 443 **Lipidomic Analyses of CEACAM1 Knockout Mouse Liver and Adipose Tissue**; Gabriel Gugui¹; Deirdre La Placa¹; Zhifang Zhang¹; John E. Shively¹; ¹City of Hope, Duarte, CA
- MP 444 **Multiclass Lipid Profiling Using Liquid Chromatography High Resolution Mass Spectrometry with Dielectric Barrier Discharge Ionization**; Felipe J Lara-Ortega¹; José Robles-Molina¹; Bienvenida Gilbert-López²; Juan F García-Reyes³; Antonio Molina-Díaz¹; Alexander Schütz⁴; Sebastian Brandt⁴; Joachim Franzke⁴; ¹University of Jaen, Jaen, Es; ²Csic-Cial, Madrid, Es; ³University of Jaen, Jaen, Andalusia; ⁴Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany
- MP 445 **Comparison of Different Stationary Phases for Gangliosides Separation**; Ashta Lakshmi Prasad Gobburi¹; Renliang Zhang²; Denise Inman³; Anderson J David⁴; ¹Cleveland State University, Department of Chemistry, Cleveland, OH; ²Cleveland Clinic Lerner Research Institute, Cleveland, OH; ³Northwest Ohio Medical University, Rootstown, Ohio; ⁴Cleveland State University, Department of Chemistr Cleveland, OH
- MP 446 **High Throughput Solid Phase Microextraction: A New Alternative for Lipid Analysis and Cellular Lipidomics**; Afsoon Pajand Birjandi¹; Vincent Bessonneau¹; Pawliszyn Janusz¹; ¹University of Waterloo, Waterloo ON, Canada
- MP 447 **Characterization of Triglycerides and Lipogenesis of Serum Lipids from Dietary or Hepatic Origin: A LC-MS/MS and GC/MS Stable-Isotope Tracer Approach**; Sergiu P Paliu¹; Grace M Jones²; Russell Caccavello¹; Alejandro Gugliucci¹; Jean-Marc Schwarz^{2,3}; ¹Department of Research, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; ²Department of Basic Sciences, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; ³Department of Medicine, University of California San Francisco, San Francisco, CA
- MP 448 **Steroid Profiling Method for Rat Serum and Plasma by Gas Chromatography/Tandem Mass Spectrometry with Large Volume Injection**; Udi Jumhawan¹; Toshiyuki Yamashita²; Motonao Nakao¹; Kuniyo Sugitate³; Takeshi Serino³; Ryoichi Sasano⁴; Yoshihiro Izumi¹; Takeshi Bamba⁵; ¹Kyushu University, Fukuoka, Japan; ²Osaka University, Suita, Japan; ³Agilent Technologies Co. Ltd, Hachioji, Japan; ⁴AIST SCIENCE CO., Ltd., Wakayama, Japan; ⁵Kyushu University, Fukuoka, Fukuoka
- MP 449 **Unsaturated Cholesteryl Ester Analysis from Human Plasma via Online Photochemical Reaction and nanoESI-MS/MS**; Jia Ren¹; Elissia Franklin¹; Yu Xia¹; ¹Purdue University, West Lafayette, IN
- MP 450 **Discovery of Endocannabinoids by Untargeted All-Ions Fragmentation High Resolution LC-MS/MS Screen**; Mesut Bilgin^{1,2}; Petra Born²; Fezza Filomena^{3,4}; Michael Heimes⁵; Nicolina Mastrangelo⁶; Nicolai Wagner²; Carsten Schultz⁵; Mauro Maccarrone^{6,7}; Suzanne Eaton²; Andre Nadler²; Matthias Wilm⁸; Andrej Shevchenko²; ¹Danish Cancer Society Research Center, Copenhagen, DK; ²Max Planck Institute for Cell Biology and Genetics, Dresden, DE; ³Department of Experimental Medicine and Surgery, University of Rome Tor Vergata, Rome, IT; ⁴European Center for Brain Research/Fondazione Santa Lucia, Rome, IT; ⁵European Molecular Biology Laboratory (EMBL), Heidelberg, DE; ⁶Department of Medicine, Campus Bio-Medico University of Rome, Rome, IT; ⁷European Center for Brain Research/Fondazione Santa Lucia, via del Fosso di Fiorano 65, Rome, IT; ⁸Conway Institute of Biomolecular and Biomedical Research, University College Dublin, Dublin, IE
- MP 451 **Role of Ammonium Salts in the Ionization and Fragmentation of Phosphatidylcholines Found in Krill Oil**; Michael Rush¹; Richard van Breemen¹; ¹University of Illinois College of Pharmacy, Chicago, IL
- MP 452 **Determination of β-Glucocerebrosidase (GBA) Activity through Global and Targeted Lipid Profiling**; Yi Zeng¹; Sangwon Min¹; Baris Bingol¹; Wendy Sandoval¹; ¹Genentech Inc, South San Francisco, CA
- MP 453 **Separation of Metalated Lipid Isomers Using Linear and Nonlinear Ion Mobility Spectrometry**; Andrew Bowman¹; Julia Kaszycki²; Rinat Abzalimov³; Gordon A Anderson⁴; Alexandre A Shvartsburg²; ¹Wichita State University, Wichita, KS - Kansas; ²Wichita State University, Wichita, KS; ³City University of New York, New York City, NY; ⁴GAA Custom Engineering, LLC Benton, WA
- MP 454 **Analysis of Lipids from Biological Samples by Laser Desorption Ionization from Silicon Nanopost Arrays**; Andrew Korte¹; Akos Vertes¹; ¹George Washington University, Washington, DC
- MP 455 **Polar Lipids from Insect and Tick Cuticle. Analysis and Discovery of their Roles in Semiochemical Signaling**; Robert Renthal; ¹University of Texas at San Antonio, San Antonio, TX
- MP 456 **Natural Variation of Blood Plasma Lipids in Healthy Asian Individuals**; Husna Begum^{1,2}; Federico Torta³; Pradeep Narayanaswamy³; Piyushkumar Mundra²; Yik-Ying Teo⁴; Peter Little¹; Peter Meikle²; Markus Wenk^{1,3}; ¹Life Sciences Institute, National University of Singapore,



Singapore, Singapore; ²Baker IDI Heart and Diabetes Institute, Melbourne VIC, Australia; ³Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore; ⁴Saw Swee Hock School of Public Health, National University of Singapore, Singapore, Singapore

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- MP 457 **Validating the Roles of FraD and FraB in the Metabolism of F-Asn by Salmonella**; Jikang Wu¹; Anindita Sengupta¹; Anice Sabag-Daigle¹; Pradip Biswas¹; Brian Ahmer¹; Venkat Gopalan¹; Edward Behrman¹; Vicki Wysocki¹; ¹Ohio State University, Columbus, OH
- MP 458 **Exploiting the Sensitivity of Structural Mass Spectrometry as a Next Generation Platform for Metabolomics**; Olga Gorlova¹; Conrad Wolke¹; Sean Colvin¹; Scott Miller¹; Mark Johnson¹; ¹Yale University, New Haven, CT
- MP 459 **Globally Optimized Targeted Mass Spectrometry (GOT-MS): Reliable Metabolomics Analysis with Broad Coverage**; Haiwei Gu¹; Ping Zhang¹; Jiangjiang Zhu¹; Daniel Raftery^{1,2}; ¹University of Washington, Seattle, WA; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 460 **Targeted Metabolomics to Characterize Lipopolysaccharide Biosynthetic Intermediates in Gram-Negative Bacteria in Response to Chemical and Genetic Perturbations**; William Sawyer¹; Jade Bojkovic¹; Charles R. Dean¹; Brian Y. Feng¹; Daryl L. Richie¹; David A. Six¹; Lisha Wang¹; Christopher M Rath¹; ¹Novartis Institutes for Biomedical Research, Emeryville, CA
- MP 461 **Internal Extractive Electrospray Ionization Mass Spectrometry based- Metabolomics for Lung Cancer Analysis**; Yun Li¹; Zhihao Wang¹; Qian Li¹; Yiping Wei²; Haiwei Gu¹; Huanwen Chen³; ¹East China Institute of Technology, Nanchang, China; ²Department of Cardiothoracic Surgery of Second Affiliated Hospital to Nanchang University, Nanchang, China; ³East China University of Technology, Nanchang, Mainland
- MP 462 **Study of Untargeted Metabolite Degradation in Plasma using Isotopic Ratio Outlier Analysis by uHPLC-HRMS**; Elizabeth Dhummakupt¹; Casey Chamberlain²; Chris Beecher³; Timothy Garrett²; ¹University of Florida, Gainesville, FL; ²Department of Pathology, University of Florida Gainesville, FL; ³IROA Technologies, Ann Arbor, MI
- MP 463 **A Step Forward in GC-HRAM-MS Based Metabolomics - A Novel Atmospheric Pressure GC-APCI Source Increases Quantitative and Qualitative Performance**; Christian J. Wachsmuth¹; Aiko Barsch²; Christoph Gebhardt²; Peter J. Oefner¹; Katja Dettmer¹; ¹University of Regensburg, Institute of Functional Genomics, Regensburg, Germany; ²Bruker Daltonics Ltd, Bremen, Germany
- MP 464 **Novel Strategies for the Analysis of Isotopologue and Isotopomer Fractions of Primary Metabolites in 13C Based Metabolic Flux Analysis Experiments**; Teresa Mairinger^{1,2}; Gunda Koellensperger³; Stephan Hann^{1,2}; ¹Austrian Centre of Industrial Biotechnology (acib), Vienna, Austria; ²Department of Chemistry, University of Natural Resources and Life Sciences - BOKU Vienna, Vienna, Austria; ³Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria
- MP 465 **13C-Metabolic Flux Analysis of Microbes by Using Novel Fragmentations of tert-Butyldimethylsilyl (tBDMS)-Amino Acid Derivatives with GC-MS/MS**; Nobuyuki Okahashi¹; Shuichi Kawana²; Junko Iida²; Hiroshi Shimizu¹; Fumio Matsuda¹; ¹Osaka University, Suita, Japan; ²Shimadzu Corporation, Kyoto, Japan

MP 466 **Analysis of Plasma Metabolites Using Gas-**

Chromatography Tandem Mass Spectrometry System with Automated TMS Derivatization; Shuichi Kawana¹; Yumi Unno²; Yukihiko Kudo³; Takero Sakai³; Takashi Kobayashi⁴; Shin Nishiumi⁴; Masaru Yoshida⁴; Noriyuki Ojima⁵; ¹Shimadzu Corporation, Osaka, Japan; ²Shimadzu Corporation, Kanagawa, Japan; ³Shimadzu Corporation, Kyoto, Japan; ⁴Kobe University Graduate School of Medicine, Kobe, Japan; ⁵Shimadzu Corporation, Tokyo, Japan

- MP 467 **LC-HRMS Metabolic Flux Analysis Reveals Mechanistic-Based Changes after Muscle AMPK Activation**; John Kenji Meissen¹; Russell Alan Miller²; Matt Blatnik¹; ¹Pfizer, Groton, CT; ²Pfizer, Cambridge, MA
- MP 468 **Metabolic Analysis of Single Human Cells in Different Mitotic Phases by Capillary Microsampling Electrospray Ionization Mass Spectrometry**; Linwen Zhang¹; Akos Vertes¹; ¹The George Washington University, Washington, DC
- MP 469 **Evaluating the Impact of Environmental Ultrafine Particles to Gut Bacterial Metabolism by targeted LC-MS/MS Metabolic Profiling**; Julia Roubidoux¹; Katie Schelli¹; Joshua Rutowski¹; Britt Holmén²; Jiangjiang (Chris) Zhu¹; ¹Department of Chemistry and Biochemistry, Miami University, Oxford, OH; ²Civil & Environmental Engineering, School of Engineering, University of Vermont, Burlington, VT
- MP 470 **Ion-pairing LC-MS with Automated Sample Prep for Metabolomics**; Jason L. Richardson¹; Bhavana Shah¹; Zhongqi Zhang¹; ¹Amgen, Inc., Thousand Oaks, CA
- MP 471 **Application of Data-Dependent MS/MS in Structural Analysis of Isomeric Acylsugar Metabolites from Solanaceous Plants**; Xiaoxiao Liu¹; 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
- MP 472 **Probiotic Lactobacillus Reuteri Strains Produce L-Ethionine via a Two-Carbon-Transferring Alternative Branch of the Folate Cycle**; Daniel Röth¹; Abby J Chiang¹; Gabriel Gugiu¹; James Versalovic²; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Texas Children's Hospital, Baylor College Houston, TX
- MP 473 **Using Isotopic Ratio Analysis (IROA) and Non-negative Matrix Factorization (NMF) to Sort Mixtures in Metabolomic Analyses**; Chris Beecher¹; Timothy J Garrett²; Elizabeth Dhummakupt²; Vanessa Y. Rubio²; ¹IROA Technologies, Gainesville, Florida; ²University of Florida, Gainesville, FL
- MP 474 **MS Profiling of Molecular Composition Inside live 3D Artificial Tumors Using the Single-Probe Device**; Wei Rao¹; Ning Pan¹; Haiqing Yu¹; Xuewei Qu¹; Chuanbin Mao¹; Zhibo yang¹; ¹University of Oklahoma, Dept. of Chem & Biochem Norman, OK
- MP 475 **5a-Reductase Type 3 (SRD5A3) Δ 4-3-keto Steroid Metabolism Using Triple Quadrupole Mass Spectroscopy**; sumankalai ramachandran; Department of Genitourinary Medical Oncology, David H. Koch Center for Applied Research of Genitourinary Cancers, The University of Texas MD Anderson Cancer Center, Houston, Texas., Houston, TX
- MP 476 **LC-SWATH/MS Metabolomics Platform with Hyphenation of Extraction and Analysis of Polar and Non-Polar Metabolites in Plasma and Urine**; Michel Raetz¹; Renzo Picononi²; Guenter Boehm²; Gerard Hopfgartner¹; ¹University of Geneva, Geneva, Switzerland; ²CTC Analytics AG, Zwingen, Switzerland
- MP 477 **What Are We Eating? Differential Metabolomic Profiles Reveal an Insight into our Dietary Habits**; Paul Clemens¹; Baljit Ubhi¹; ¹SCIEX, Redwood City, CA

- MP 478 **Molecular Network Analysis of Environmental Samples for Drug Discovery;** Stefano Bonissone¹; Natalie E Castellana¹; ¹Digital Proteomics, LLC. San Diego, CA
- MP 479 **Labeling of Specialized Metabolites in the Medicinal Plant *Camptotheca acuminata* using ¹³CO₂ to Track Intermediates in the Biosynthetic Pathway;** Sujana Pradhan¹; Daniel A Jones²; Zhenzhen Wang²; ¹Michigan State University, Haslett, MI; ²Michigan State University, East Lansing, MI
- MP 480 **Development of an LC-MS Method for the Kinetic Flux Profiling of a Diverse Set of Metabolic Pathways;** Jay Kirkwood^{1,2}; Corey Broeckling^{1,2}; Jordan Steel^{1,3}; Becky Gullberg^{1,3}; Rushika Perera¹; Jessica Prenni^{1,2}; ¹Colorado State University, Fort Collins, CO; ²Proteomics and Metabolomics Facility, Fort Collins, Colorado [CO]; ³Arthropod-borne & Infectious Diseases Laboratory, Fort Collins, CO
- MP 481 **$\Delta 9$ -THC Metabolites and Other Cannabinoid Detection;** Toshi Ono¹; Ken Tseng²; Tsunehisa Hirose³; ¹Nacalai USA, San Diego, CA; ²Nacalai USA Inc., San Diego, CA - California; ³Nacalai Tesque Inc., Kyoto, Japan
- MP 482 **Determining Pentose Phosphate Pathway Metabolism in VHL (-) Clear Cell Renal Carcinoma (ccRCC);** Collin Wetzel¹; Megan Bischoff¹; Johnson Chu¹; Patrick A Limbach¹; David R Plas¹; Maria F Czyzyk-krzeska¹; ¹University of Cincinnati, Cincinnati, OH
- MP 483 **An Optimized Acquisition Database and LC-MS/MS Method Targeting Central Carbon Pathway Metabolites;** Mark Sartain¹; Amy Caudy^{2,3}; Adam Rosebrock^{2,3}; ¹Agilent Technologies, Santa Clara, CA; ²Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto ON, Canada; ³Department of Molecular Genetics, University of Toronto, Toronto ON, Canada
- MP 484 **Lanthanide-Chelator Barcode for Combinatorial Screening Applications;** Todd Duncombe¹; Kai Deng¹; Paul D Adams²; Anup K Singh¹; Trent R Northen²; ¹Sandia National Laboratories, Albuquerque, NM; ²Lawrence Berkeley National Lab, Berkeley, CA
- MP 485 **Chromatographic performance for high resolution metabolomics;** Vilinh Tran^{1,2}; Ken Liu^{1,2}; Dean Jones^{1,2}; ¹Clinical Biomarker, Emory School of Medicine Atlanta, GA; ²Emory University School of Medicine, Atlanta, GA
- MP 486 **Development of Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Metabolomic Analysis of Small Numbers of Mammalian Cells;** Xian Luo¹; Liang Li²; ¹University of Alberta, Edmonton, Alberta; ²University of Alberta, Edmonton, Canada
- MP 487 **Cow Milk Metabolome Profiling and Determination of its Dietary Effects on the Human Urine Metabolome Using Chemical Isotope Labeling LC-MS;** Dorothea Mung¹; Liang Li¹; ¹University of Alberta, Edmonton, Canada
- MP 488 **Metabolic Profiling of Human Sweat from Various Epidermal Locations Using Non-occlusive Sample Collection and Chemical Isotope Labeling LC-MS;** Kevin Hooton¹; Liang Li¹; ¹University of Alberta, Edmonton, Canada
- MP 489 **Metabolic Phenotyping of Platelet-Rich Plasma Using the AbsoluteIDQ™ p180 kit;** Lisa St John Williams¹; Guido Dallmann²; Will J Thompson¹; Therese Koal²; ¹Duke University Medical Center, Durham, NC; ²Biocrates Life Science AG, Innsbruck, Austria
- MP 490 **Metabolomic Analysis of ¹³C/¹⁵N Labeled Metabolites Utilizing High Resolution Orbitrap™ Mass Spectrometry and Compound Discoverer Software;** Anastasia Kalli¹; Bryson Bennett²; Junhua Wang¹; Caroline Ding¹; Ralf Tautenhahn¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Calico Labs, South San Francisco, CA
- MP 491 **Development of Ion Pair-Reverse Phase Chromatography Mass Spectrometry Method to Maximize Isomer Separation and Coverage of Endogenous Metabolite Classes;** Yugin Dai; Agilent Technologies, Santa Clara, CA
- MP 492 **Formate Tetrahydrofolate Ligase of *Lactobacillus reuteri*: A Multifaceted Player of the Folate Cycle?;** Abby Chiang¹; Daniel Röth¹; James Versalovic²; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Texas Children's Hospital, Baylor College Houston, TX
- MP 493 **Development of MRM-Based Detection of the Plant Metabolome Using Liquid Chromatography/Tandem Mass Spectrometry;** Satoshi Yamaki¹; Junichi Masuda²; Yoshihiro Hayakawa³; Muneo Sato⁴; Yuji Sawada⁴; Masami Yokota Hirai⁴; ¹Shimadzu Corporation, Kanagawa, E; ²Shimadzu Corporation, Kanagawa, Japan; ³Shimadzu Corporation, Kyoto, Japan; ⁴RIKEN, Yokohama, Japan
- MP 494 **Fractionation and Untargeted Metabolomics of Human Plasma by Off-Line Coupling of Reversed-Phase and Hydrophilic Interaction Liquid Chromatography LC/MS;** Stefanie Wernisch¹; Subramaniam Pennathur^{1,2}; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan Medical School, Ann Arbor, MI
- MP 495 **Wine Flavonoids Identified and Analyzed by Composite Neutral Loss Scan and Novel Data-Dependent Scans for Metabolomics Discovery by LC/MS/MS;** Bennett Kalafut¹; Rae Ana Snyder¹; Mark Dreyer¹; ¹Thermo Fisher Scientific, San Jose, CA

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- MP 496 **Utility of Random Forest Combined with Infusion Electrospray MS and MALDI-TOF MS for Rapid Classification of *Neisseria Meningitidis* Strains;** Adrian R Woolfitt¹; Hercules Moura¹; Bryan A Parks¹; Ramnath Gowrishankar¹; Conrad P Quinn¹; Brian H Harcourt¹; Xin Wang¹; John R Barr¹; ¹CDC, Atlanta, GA
- MP 497 **Identification of Microorganisms in Biofluids and Saliva of Individuals with Periodontitis and Chronic Kidney Disease Using MALDI Biotyper;** Levy Anderson Cesar Alves¹; Rafael Celestino Souza¹; Taciana Mara Couto Silva¹; Marcelo Fava²; Meriellen Dias³; Maria Anita Mendes³; Ana Lidia Ciamponi¹; ¹Orthodontics and Paediatric Department – Dental School – University of São Paulo, Sao Paulo, SP - BR; ²Paediatric Nephrology Department – Medical School – University of São Paulo (USP), Sao Paulo, SP/BRAZIL; ³LSCP - Chemical Engineering Department - Polytechnics School – University of São Paulo (USP), Sao Paulo, SP/ Brazil
- MP 498 **A Peptide-Based LC-MS/MS Method for Detection and Identification of *Salmonella* serovars;** Shu-Hua Chen¹; Christine H. Parker¹; Melinda A. McFarland¹; Timothy R Croley¹; ¹FDA/CFSAN, College Park, MD
- MP 499 **Detection of Penicillin Binding Protein 2a for the Identification of Methicillin Resistant *S.aureus* Using Top-down Proteomics;** Jason Neil¹; James Jr L Stephenson²; Alexander Cherkassky³; ¹Thermo Fisher Scientific, Cambridge, MA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose CA, CA
- MP 500 **Reliable Biomarkers for Identification of *Mycobacterium Tuberculosis* Complex in Broth Culture Media with Nanodiamond;** Hsi-An Chen¹; Ya-Chin Chin¹; Po-Chi Soo²; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng Hualien, Taiwan; ²Tzu Chi University, Hualien, Taiwan
- MP 501 **Deciphering Multifactorial Resistance in *Acinetobacter baumannii* Combining Whole-Genome Sequencing and Targeted Label-Free Proteomics;** Tiphaine Cecchini¹; Eun-Jeong Yoon²; Corinne Beaulieu¹; Yannick Charretier¹; Chloe Bardet¹; Xavier Lacoux¹; Zack Blair³; Patrice Courvalin²;



- Jerome Lemoine⁴; Catherine Grillot-Courvalin²; Jean-Philippe Charrier¹; ¹Biomérieux, Marcy L'Etoile, France; ²Institut Pasteur, Paris, France; ³bioMérieux, Saint Louis, Missouri; ⁴ISA, Unit 5280 CNRS/UCBL-1 Villeurbanne, France
- MP 502 **Novel Genetic Determinants for Complex Head Composition in a Giant Salmonella Phage**; Susan T. Weintraub¹; Adriana Coll²; Martine Bosch²; Kevin Hakala³; Sammy Pardo¹; Dana Molleur¹; Stephen C Hardies¹; Lindsay W Black⁴; Julie A Thomas²; ¹Univ. of Texas HSC, San Antonio, TX; ²Rochester Institute of Technology, Rochester, NY; ³Thermo Fisher Scientific, San Jose, CA; ⁴University of Maryland School of Medicine, Baltimore, MD
- MP 503 **Thermal Desorption Electrospray/Ionization Mass Spectrometry Combined with Principal Component Analysis for Rapid Characterization of Bacterial Species**; Shiang Jiun Lin¹; Sung Pin Tseng²; Hung Su¹; Yang Kuang Pan¹; Jentaie Shiea¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Kaohsiung Medical University, Kaohsiung, Taiwan
- MP 504 **Application of Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry for Differentiation of Cacao Phytopathogen Strains Growing in Different Tissues and Hosts**; Fábio Santos¹; Alessandra Tata¹; Kátia Belaz¹; Dilze Magalhães²; Edna Luz²; Marcos Nogueira Eberlin¹; ¹University of Campinas, Campinas SP, Brazil; ²CEPLAC, Ilhéus Bahia, Brazil
- MP 505 **MALDI Profiling of Cyanobacteria by Monitoring Large Molecules**; Hirohiko Asukabe¹; Takuma Nakayama¹; Ken-ichi Harada¹; Susumu Y. Imanishi²; ¹Meijo University, Nagoya, Japan; ²Meijo University, Nagoya, Aichi
- MP 506 **Identification of Fungi using Rapid Evaporative Ionisation Mass Spectrometry**; Frances Bolt¹; Simon Cameron¹; Ali Abdolrasouli¹; Johanna Rhodes¹; Tony Rickards²; Kate Hardiman¹; Adam Burke¹; Julia Balog³; Tamas Karancsi³; Daniel Simon³; Richard Schaffer³; Zsolt Bodai¹; Monica Rebec²; Zoltan Takats¹; ¹Imperial College, London, United Kingdom; ²Imperial College Healthcare Trust, London, UK; ³Waters Research Center, Budapest, Hungary
- MP 507 **Identification and Species Delineation of Bacteria Using MALDI-TOF MS Based on Ribosomal Protein Sequences in DNA Databases**; Kenneth Parker; SimuTOF/ VIC Instruments, Marlborough, MA
- MP 508 **Differentiation of Bacteria at the Strain Level by MALDI-MS of Proteins >15kDa**; Franco Basile¹; Anthony Maus¹; Bledar Bisha¹; ¹University of Wyoming, Laramie, WY
- MP 509 **Liquid Extraction Surface Analysis Mass Spectrometry for Protein Analysis Directly from *Escherichia coli* and *Staphylococcus epidermidis***; Klaudia I Kocurek^{1,2}; Josephine Bunch²; Robin C May¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²National Physical Laboratory, Teddington, United Kingdom
- MP 510 **High-velocity Impact Survival and Bouncing Kinetics of Electrosprayed Bacterial Spores Studied using Novel Asymmetric Image Charge Detectors**; Brandon Barney¹; Daniel Austin¹; ¹Brigham Young University, Provo, UT
- MP 511 **Probing Protein Interaction Dynamics between Asian Citrus Psyllid and *Candidatus Liberibacter asiaticus* by Chemical Crosslinking Mass Spectrometry**; Xuefei Zhong¹; John Ramsey^{2,3}; Juan Chavez¹; Arti Navare¹; Jared Mohr⁴; Michelle Cilia^{2,3,4}; James Bruce¹; ¹University of Washington, Seattle, WA; ²USDA Agricultural Research Service, Ithaca, NY; ³Boyce Thompson Institute for plant research, Ithaca, NY; ⁴Cornell University, Ithaca, NY
- MP 512 **High Yielding Spin Column Isolation of Total Proteins from Microbial Cultures for Proteomic Applications**; Victoria Nieciecki¹; Heather Callahan¹; Eddie Adams²; ¹MO BIO Laboratories, Carlsbad, CA - California; ²MO BIO Laboratories, Carlsbad, CA
- MP 513 **Simultaneous DNA, RNA, and Protein Extraction from Microbial Cells: Sequential Isolation of Complex Biomolecules from a Single Source**; Heather Callahan¹; Victoria Nieciecki¹; Eddie Adams¹; ¹MO BIO Laboratories, Carlsbad, CA
- MP 514 **Characterizing the Formation of Electrophilic Fatty Acid Derivatives During Influenza Infection and Determining their Role in Pathogenesis**; Greg Buchan; University of Pittsburgh, Pittsburgh, PA
- MP 515 **Integrated Omics Reveals Dynamic Nature of the Arabidopsis Rhizosphere Microbiome**; Ljiljana Pasa-Tolic¹; Abigail Ferrieri²; Charles K. Ansong²; Heather M. Brewer²; Angela D. Norbeck²; Yaya Cui³; Christopher Staley⁴; Malak Tfaily²; Rosalie Chu²; Jared Shaw²; Meng L. Markillie²; Richard A. Ferrieri³; Susannah G. Tringe⁵; Michael J. Sadowsky^{4,6}; Gary Stacey³; ¹Battelle - PNNL, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA; ³University of Missouri, Columbia, MO; ⁴University of Minnesota, St. Paul, MN; ⁵DOE Joint Genome Institute, Walnut Creek, CA; ⁶University of Minnesota at Twin Cities, Saint Paul, MN
- MP 516 **Development of Metaproteomics Methods for Characterization of Soil Microbial Communities**; ZHOU LI¹; Cristina N. Butterfield²; Susan Spaulding²; Brian C. Thomas²; Andrea Singh²; K. Blake Suttle³; Robert Hettich¹; Jillian Banfield²; Chongle Pan¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of California, Berkeley, CA; ³University of California, Santa Cruz, Santa Cruz, CA
- MP 517 **Non-Targeted Mass Spectrometry-based Analysis for the Differentiation of Pathogenic *Escherichia coli* Strains**; Rabih Jabbour¹; Raja Sekhar Nirujogi²; Kim Min-Sik³; Mary M Wade⁴; Babylakshmi Muthusamy⁵; Gajanan J. Sathe⁵; T.S. Keshava Prasad^{6,7}; Akhilesh Pandey^{3,8}; ¹ECBC, APG, MD; ²Institute of Bioinformatics, International Technology Park, Bangalore, India; ³McKusick-Nathans Institute of Genetic Medicine, Johns Hopkins University School of Medicine, Baltimore, MD; ⁴ECBC, Apg, MD; ⁵Institute of Bioinformatics, Bangalore, India; ⁶Institute of Bioinformatics, Bangalore, India; ⁷Centre for Bioinformatics, Pondicherry University, Puducherry, India; ⁸Department of Biological Chemistry, Pathology, Oncology, Johns Hopkins University School of Medicine, Baltimore, MD

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- MP 518 **Enrichment and Identification of MHC-Associated Phosphopeptide Neoantigens in Hepatocellular Carcinoma for the Development of Novel Cancer Immunotherapeutics**; Paisley Myers¹; Nico Buttner²; Jennifer G Abelin¹; Sarah A. Penny²; Lora G Steadman²; Dina L. Bai¹; Mark Cobbold³; Jeffrey Shabanowitz¹; Donald F Hunt¹; ¹University of Virginia, Charlottesville, VA; ²University of Birmingham, Birmingham, UK; ³Harvard University, Boston, MA
- MP 519 **Phosphoproteome Changes in Altered Cholesterol Metabolism Revealed by SCX Tip Based Fractionation of Batch-Enriched Phosphopeptides**; Alireza Dehghani¹; Markus Gödderz¹; Volkmar Gieselmann¹; Dominic Winter¹; ¹University of Bonn, Bonn, Germany
- MP 520 **Development of Enrichment Strategies for the Analysis of Phosphohistidine-Containing Peptides**; Gemma E Hardman¹; Claire E Eyers¹; ¹University of Liverpool, Liverpool, United Kingdom
- MP 521 **Enrichment of Phosphorylated Peptides Using Metal-Loaded Polymeric Reverse Micelles for MALDI-MS Analysis**; Meizhe Wang¹; Bo Zhao¹; Sankaran Thayumanavan¹; Richard Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA

- MP 522 **Fabrication of MnFe₂O₄ Magnetic Nanoparticles for the Enrichment of Phosphopeptides in Combination with Mass Spectrometric Analysis;** Yung-Yun Huang¹; He-Hsuan Hsiao²; ¹*Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan;* ²*Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan*
- MP 523 **Dual Wield nanoLC-ESI-MS for Simultaneous Detection of Singly and Multiply Phosphorylated Peptides;** Chia-Feng Tsai¹; Kosuke Ogata¹; Masaki Wakabayashi¹; Naoyuki Sugiyama¹; Yasushi Ishihama¹; ¹*Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan*
- MP 524 **Metal Ion-Immobilized Magnetic Nanoparticles for Global Enrichment and Identification of Phosphopeptides by Mass Spectrometry;** Yangjun Zhang^{1,2}; Rui Zhai²; XiaoHong Qian²; ¹*Beijing Proteome Research Ctr, Beijing, Beijing;* ²*Beijing Institute of Radiation Medicine, Beijing, C.N.*
- MP 525 **Excellent Sensitivity through Excellent Recovery – ERLIC Outperforms TiO₂-Affinity Purification in Quantitative Phosphoproteomics with Low Sample Amounts;** Stefan Loro¹; Albert Sickmann^{1,2,3}; René P Zahedi¹; ¹*Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany;* ²*Ruhr-Universität-Bochum, Medizinische Fakultät, Bochum, Germany;* ³*University of Aberdeen, School of Natural & Computing Sciences, Aberdeen, Scotland*
- MP 526 **ESI Tandem Mass Spectrometric Analysis of Phosphopeptide Modified by Cyclic Quaternary Ammonium Tags;** Hye Kyong Kweon¹; Kristina Hakansson¹; Philip Andrews¹; ¹*University of Michigan, Ann Arbor, MI*
- MP 527 **Method Development and Evaluation of the Protein Phosphatase 2 Phosphoproteome Using the Chip iFunnel QTOF Platform;** Brooke Thompson¹; Vadiraja Bhat²; Chelsea E. Cunningham³; Paulos Chumala¹; Frederick S. Vizeacoumar³; Franco J. Vizeacoumar³; George S. Katselis¹; ¹*CCHSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada;* ²*Agilent Technologies, Wilmington, DE;* ³*Department of Pathology, Cancer Cluster, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada*
- MP 528 **Acid-Based SCX Fractionation for In-Depth Proteome and Phosphoproteome Analysis;** Jun Adachi¹; Hashiguchi Kazunari²; Nagano Maiko²; Sato Misako²; Sato Ayako²; Fukamizu Kazuna²; Ishihama Yasushi³; Tomonaga Takeshi²; ¹*National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Osaka;* ²*National Institute of Biomedical Innovation, Health and Nutrition, Osaka, Japan;* ³*Kyoto University, Kyoto, Japan*
- MP 529 **Two-Step Elution of Phosphopeptides from TiO₂ Microparticles – an Improved Detection of Multiphosphorylated Peptides;** Rudolf Kupcik¹; Pavel Rehulka²; Ivo Fabrik²; Jana Klimentova²; Helena Rehulkova²; Jiri Stulik²; Pavla Krulisova¹; Zuzana Bilkova¹; ¹*Department of Biological and Biochemical Sciences, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic;* ²*Department of Molecular Pathology and Biology, Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech Republic*
- MP 530 **Characterization of Bromine Functionalized Alternating and Random Copolyesters by Tandem Mass Spectrometry;** Selim Gerislioglu¹; Xianglin Yin²; Coleen Pugh²; Chrys Wesdemiotis²; ¹*The University of Akron, Akron, Ohio;* ²*The University of Akron, Akron, OH*
- MP 531 **The Characterization of Polymeric Methylene Diphenyl Diisocyanates (PDMIs) Using UHPSC and FT-ICR APPI-MS;** Julie M Herniman¹; Robert Carr²; John G Langley¹; ¹*University of Southampton, Southampton, United Kingdom;* ²*Huntsman (Europe), bvba, Everborg, Belgium*
- MP 532 **An APCI LC-MS-MS Method for the Determination of Octamethylcyclotetrasiloxane (D4), Decamethylcyclopentasiloxane (D5), and Dodecamethylcyclohexasiloxane (D6) in Silicone Emulsions.;** Ron Tecklenburg¹; Tanya M Habitz¹; ¹*Dow Corning Corporation, Auburn, MI*
- MP 533 **Simplification of Polysorbate 80 Spectrum: Selective Removal of Metal Cation Adducts from Polymers via Gas-Phase Ion/Ion Reactions Using Carborane Anions;** Stella Betancourt¹; Alice L Pilo¹; Jiexun Bu¹; Scott A McLuckey¹; ¹*Purdue University-Department of Chemistry, West Lafayette, IN*
- MP 534 **Self-Assembly and Characterization of 2D to 3D Supramolecular Star of David Using Mass Spectrometry;** Bo Song¹; Xiaopeng Li¹; Ming Wang¹; ¹*Texas State University, San Marcos, TX*
- MP 535 **Analysis for Extractable and Leachable Compounds from Polymeric Materials;** Gordon Fujimoto¹; Sarah Dowd¹; Baiba Cabovska²; Marian Twohig²; ¹*Waters Corporation, Beverly, MA;* ²*Waters Corporation, Milford, MA*
- MP 536 **Identification of Poly Ethylene Glycol (PEG) and PEGylated Detergents Using Protein Search Engines;** Shiva Ahmadi¹; Dominic Winter¹; ¹*University of Bonn, Bonn, Germany*
- MP 537 **Assembling and Characterization of Discrete Supramolecular Fractal Architectures Using ESI-MS and Ion Mobility-Mass Spectrometry ;** Yuanfang Ying¹; Ming Wang¹; Kendall Williams¹; Xiaopeng Li¹; ¹*Texas State University, San Marcos, TX*
- MP 538 **Mass Spectrometry Characterization of Isomeric Biodegradable Polyesters;** sahar sallam¹; Chrys Wesdemiotis¹; Yuanyuan Luo¹; Mathew L. Becker¹; ¹*The University of Akron, Akron, OH*
- MP 539 **Surface Composition of Films Made from Partially Functionalized Polymer Blends;** Kevin Endres¹; Jacob A. Hill¹; John Meyerhofer²; Qiming He¹; Chrys Wesdemiotis¹; Mark D Foster¹; ¹*The University of Akron, Akron, OH;* ²*Saint Vincent College, Latrobe, PA*
- MP 540 **MALDI-MS Signal Enhancement of Peptides from Donor-Acceptor Interactions between Amphiphilic Polymers and MALDI Matrix;** Mahalia Serrano¹; Huan He¹; Sankaran Thayumanavan¹; Richard W Vachet¹; ¹*University of Massachusetts Amherst, Amherst, Massachusetts*
- MP 541 **Investigating the Effect of Sample Preparation Parameters on the Cationization of Synthetic Polymers Using Matrix-Assisted Laser Desorption Ionization;** Michelle Piotrowski¹; Kevin Owens¹; ¹*Drexel University, Philadelphia, PA*
- MP 542 **Revealing Topological Isomers Inside Insoluble Cyclo-Para-Phenylenes by Ion Mobility Mass Spectrometry;** Hans Joachim Raeder¹; Wen Zhang²; Ali Abdulkarim²; Klaus Müllen²; ¹*MPI for Polymer Research, Mainz, Rhineland-Palatinate;* ²*MPI for Polymer Research, Mainz, Germany*
- MP 543 **Matrix Assisted Laser Desorption Ionization Mass Spectrometry and NMR Characterization of Plasma Polymerized Styrene;** Lee Elliott¹; Kris Micheal Kirmess¹; Gary Ray Kinsel¹; ¹*Southern Illinois University Carbondale, Carbondale, IL*
- MP 544 **Highly Sensitive Analysis of Residual Monomers in Adhesives Using HSGC/MS;** Sanket Chiplunkar¹; Durvesh Sawant²; Dheeraj Handique¹; Prashant Hase¹; Ankush Bhone¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; ¹*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, Maharashtra;* ²*Shimadzu Analytical (India) Pvt. Ltd.,*

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- MP 545 **Polymer and Adhesive Tape Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time (DART) Mass Spectrometry;** Cody Robert B. ¹; Chikako Takei²; Haruo Shimada³; Yasuo Shida⁴; Akihiko Kusai⁵; ¹JEOL USA, Inc. Peabody, MA; ²BioChromato, Inc. Fujisawa, Japan; ³Shiseido Research Center, Yokohama, Japan; ⁴University of Yamanashi, Kofu, Japan; ⁵JEOL Ltd., Akishima, Japan
- MP 546 **Polymer Structure Investigation by Trapped Ion Mobility Mass Spectrometry;** Jan Jordens¹; Ynze Mengerink¹; Esra Altuntas¹; Mark E Ridgeway²; Melvin Park²; Maarten Honing^{1,3}; ¹DSM Resolve, Geleen, Netherlands; ²Bruker Daltonic, Billerica, MA; ³VU University, Amsterdam, Netherlands
- MP 547 **Improved Characterization of Complex Mixtures via Liquid Chromatography/Charge Reduction/Mass Spectrometry (LC/CR/MS);** John Stutzman¹; Matthew C Crowe²; James IV N Alexander²; Bruce Bell¹; Melissa N Dunkle³; ¹The Dow Chemical Company, Midland, MI; ²The Dow Chemical Company, Collegeville, PA; ³The Dow Chemical Company, Terneuzen, NL
- MP 548 **Characterization of Unknown Surfactant Packages in Industrial Samples by Liquid Chromatography Mass Spectrometry (LC/MS) with Electrospray Ionization (ESI);** Dale Willcox¹; Noelle Elliott¹; ¹Intertek, Allentown, PA

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- MP 550 **Protein Mass Spectra Database for Rapid Identification of Field-Caught Phlebotomine Sand Flies;** Kristyna Hlavackova¹; Daniel Kavan²; Vit Dvorak¹; Petr Volf¹; Petr Halada²; ¹Department of Parasitology, Charles University in Prague, Prague, Czech Republic; ²Institute of Microbiology CAS, Prague, Czech Republic
- MP 551 **Developments in Analysis of GPCRs: Monitoring Protein Movement by Means of Mass Spectrometry;** Krzysztof Okrasa¹; James Errey¹; Rob Cooke¹; ¹Heptares Therapeutics Ltd., Welwyn Garden City, UK
- MP 552 **Improving the Efficiency and Rapidity of Tryptic Proteolysis: from Blood to "Unknown Stains";** Ektá Patel¹; Paola Cicatiello²; Lisa Deininger¹; Malcolm R Clench¹; Peter Marshall³; Andy West³; Simona Francese¹; ¹Centre for Mass Spectrometry Imaging, Biomolecular Research Centre, Sheffield, South Yorkshire; ²Università di Napoli Federico II, Dipartimento di Scienze Chimiche, Naples, Naples; ³GlaxoSmithKline, Stevenage, UK
- MP 553 **How Sequence Variant Analysis can be Hampered by Trypsin Side Reactions;** Georg Drabner¹; Marco Boettger¹; ¹Roche Innovation Center Penzberg, Penzberg, Germany
- MP 554 **Mass spectrometry of Collagen and Casein in the Remains of the 5th to 7th Century Bamiyan Buddhas;** Takashi Nakazawa¹; Kazuki Kawahara²; Shunsuke Fukakusa³; Mao Karino³; Miho Takashima⁴; Yoko Taniguchi⁵; ¹Nara Women's University, Nara, Nara; ²Osaka University, Suita, Japan; ³Nara Women's University, Nara, Japan; ⁴The National Museum of Western Art, Tokyo, Japan; ⁵University of Tsukuba, Tsukuba, Japan
- MP 555 **Proteomic Characterization of Cell Architecture and its Preparatory Biochemical Extractions;** Li-Hua Li¹; Cheng-Chih Richard Hsu²; Cheng-Hsien Yang³; Chen Meng⁴; Yeou-Guang Tsay^{3,5,6}; ¹Taipei Veterans General Hospital, Taipei, Taiwan; ²Department of Chemistry National Taiwan University, Taipei, Taiwan; ³Institute of Biochemistry and Molecular Biology, Taipei, Taiwan; ⁴Chair of Proteomics and Bioanalytics Technische Universität München, Munich, Germany; ⁵Proteomics Research Center, Taipei, Taiwan; ⁶Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan
- MP 556 **The Interactions between N-Heterocyclic Carbene Silver Complex and Cytochrome C Studied by Electrospray Ionization Mass Spectrometry;** Yan Pan¹; Morgantown, WV
- MP 557 **A Chemical Proteomic Method for the Discovery of Novel LPA-binding Proteins;** Xuejiao Dong¹; Yinsheng Wang¹; ¹University of California - Riverside, Riverside, CA
- MP 558 **Exploring the Differences in Endocytic Vesicles with the Aid of Mass Spectrometry Based Protein and Lipid Profiling;** Bini Ramachandran¹; Krishnamurthy H²; Satyajit Mayor^{3,4}; ¹National Centre for Biological Sciences, Bangalore, India, Bangalore, Karnataka; ²Centre for Imaging and Flow Cytometry Facility, National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; ³National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; ⁴Institute for Stem Cell Biology and Regenerative Medicine, Bellary Road,, Bangalore, India
- MP 559 **Quality by Design (QbD) Based Development of a Peptide Mapping UPLC Method for Recombinant Human Serum Albumin (rHSA);** Ashraf Madian¹; Irish Gibson²; Janet G. De Los Reyes³; Cassandra Norton⁴; Shen Chen⁵; Lisa Cherry²; ¹Global Technology Services, Hospira, a Pfizer Company, Lake Forest, IL; ²One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, McPherson, KS; ³Global Established Products R and D, Hospira, a Pfizer Company, McPherson, KS; ⁴Global Technical Supply, Hospira, a Pfizer Company, McPherson, KS; ⁵One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, Lake Forest, IL
- MP 560 **Using LC-MS Based Methods for Testing the Digestibility of a Non-Purified Membrane Protein in Simulated Gastric Fluid;** Wayne Skinner^{1,2}; Brett S Phinney³; Anthony Herren³; John Goodstal¹; Isabel Dicely¹; Daniel Facciotti¹; ¹Arcadia Biosciences, Davis, CA; ²Arcadia Biosciences, Davis, Davis, CA; ³Proteomics Core Facility, University of California, Davis, CA 95616, USA, Davis, CA
- MP 561 **Using UHPLC-ESI-HRMS to Detect Small Mass Differences in High Molecular Weight Glutenin Subunits of Wheat;** Ray Bacala¹; Dave Hatcher²; ¹Canadian Grain Commission, Winnipeg, MB; ²Canadian Grain Commission, Winnipeg, Canada
- MP 562 **Towards a Prediction of Protein Reactivity Against Electrophile Ligands: 1. Ranking Amino Acid Side Chain Nucleophilicities;** Guillaume Gabant¹; Yoann Richer¹; Solène Motteau¹; Emmanuelle Mebold²; Martine Cadene¹; ¹CBM CNRS UPRA301, Orleans, France; ²IMMM CNRS UMR 6283, Le Mans, France
- MP 563 **Evaluation of N-terminal Labeling Protocols for Determination of Protein Cleavage Sites by Mass Spectrometry;** Michelle Gadush¹; Maria D. Person¹; ¹University of Texas at Austin, Austin, TX
- MP 564 **Identification of Unique Rod Outer Segment Plasma Membrane Proteins Using a Label-Free Protein Correlation Profiling;** Nikolai P Skiba¹; Vadim Y Arshavsky¹; ¹Albert Eye Research Institute, Duke University Medical Center, Durham, NC

- MP 565 **Identification of Polyglutamylation of C-Terminal Tails of Tubulins from In-Gel Double Digests with Trypsin and Subtilisin**; Hang-Gyeong Chin¹; Colleen McClung¹; Sriharsa Pradhan¹; Christopher J. Noren¹; Cristian I. Ruse¹; ¹New England Biolabs, Ipswich, MA
- MP 566 **Disulfide Bond Reduction on TiBlue Electrodes – a Breakthrough in Protein Analysis**; Jean-Pierre Chervet¹; Agnieszka Kraj²; Hendrik-Jan Brouwer²; Nico Reinhoud²; Martin Eysberg³; ¹Antec, Zoeterwoude, -; ²Antec, Zoeterwoude, The Netherlands; ³Antec LLC, Boston, MA
- MP 567 **Rapid Analysis of Proteins on High-Resolution Mass Spectrometers Using Matrix-Assisted Ionization**; Shameemah Thawoos¹; Casey Daniel Foley¹; James Wager-Miller²; Ken Mackie²; Paul Stemmer¹; Sarah Trimpin¹; ¹Wayne State University, Detroit, MI; ²Indiana University Dept. Chemistry, Bloomington, IN
- MP 568 **A New Thiol Derivatization Reactions with 2,1,3-Benzotelluradiazole Studied by Mass Spectrometry**; Chang Xu¹; Qiuling Zheng¹; Kehua Xu²; Bo Tang²; Hao Chen¹; ¹Ohio University, Athens, OH; ²Shandong Normal University, Jinan, SD
- MP 569 **Native Mass Spectrometry Analysis of Membrane-Bound Reaction Center from *Blastochloris viridis***; Yue Lu¹; Zhang Hao, ¹; Michael L Gross¹; Robert E Blankenship¹; ¹Washington University in St. Louis, St. Louis, MO
- MP 570 **Improved Proteolytic Digestion under High Pressure Cycling: Rapid Digestion with Improved Sensitivity and Sequence Coverage**; Vera S. Gross¹; John Wilson²; Alexander Lazarev¹; ¹Pressure BioSciences, South Easton, MA; ²Protifi, LLC, Huntington, NY
- MP 571 **Fully Automated Digestion, Separation and Analysis of the Human Prolactin Receptor Transmembrane Protein by LC-MS/MS**; Joshua Emory¹; Nishi Rochelle¹; Boutaghou Nazim¹; Feild J Brian¹; ¹Shimadzu Scientific Instruments, Inc. Columbia
- PROTEINS: PTMS (PART 1)**
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- MP 572 **Proteomic Analysis of Protein S-Sulphydration in *Staphylococcus aureus***; Yixiang Zhang^{1,2}; Hui Peng^{1,3}; David Peter Giedroc^{1,3}; Jonathan Cyboski Trinidad^{1,2}; ¹Department of Chemistry, Indiana University, Bloomington, IN; ²Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; ³Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN
- MP 573 **Deep Coverage of the Mouse Cysteine Sulfenome in vivo**; Shin-Cheng Tzeng¹; Sjoerd Van der Post¹; Nelmi O Devarie-Baez²; Cristina M Furdai²; Jason Held¹; ¹Washington University in St. Louis, St. Louis, MO; ²Wake Forest School of Medicine, Winston-Salem, NC
- MP 574 **Quantifying Oxidation in Peptides Containing Multiple Methionine Residues**; Joshua T Shipman¹; Eden P Go¹; Heather Desaire¹; ¹University of Kansas, Lawrence, KS
- MP 575 **Quantifying Reversible Oxidation of Protein Thiols in *Arabidopsis thaliana***; Evan Mc Connell¹; Leslie M Hicks¹; ¹University of North Carolina, Chapel Hill, NC
- MP 576 **Energetics of S-Palmitoylation: Role of Proline and Neighboring Cysteines**; Neelam Khanal¹; Vikas Pejaver¹; Zhiyu Li^{1,2}; Predrag Radivojac³; David E Clemmer¹; Suchetana Mukhopadhyay³; ¹Indiana University Dept. Chemistry, Bloomington, IN; ²Novilytic, West Lafayette, IN; ³Indiana University, Bloomington, IN
- MP 577 **Elevated Level of S-Glutathionylation of Hemoglobin in Mole-Rats Determined by LC-MS**; Kuanysb Kabytaev¹; Christiane Vole²; Dmitriy Shin¹; Philip Dammann²; Alexandre Stoyanov¹; ¹Department of Pathology & Anatomical Sciences, University of Missouri, Columbia, MO; ²Department of General Zoology, University of Duisburg-Essen, Essen, Germany
- MP 578 **Difference Gel Electrophoresis for Phosphoproteomics (DiGEP)**; Mayank Srivastava¹; Linna Wang¹; Weiguo Andy Tao¹; ¹Purdue University, West Lafayette, IN
- MP 579 **Intact Phosphorylated Protein Analysis by Microfluidic CE-ESI-MS**; Esme Candish¹; Michael E Pacold²; Scott Mellors³; Michael J Ramsey¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Whitehead Institute for Biomedical Research, Cambridge, MA; ³908 Devices Inc., Boston, MA
- MP 580 **Elucidating Kinase Substrate Networks in *Chlamydomonas reinhardtii***; Alex Chao¹; Chris A Broberg¹; Megan C Connor¹; Leslie M Hicks¹; ¹UNC Chapel Hill, Department of Chemistry Chapel Hill, NC
- MP 581 **Studies of the Molecular Mechanisms in the Regulation of PRL-3 Phosphatase Activity in the Endothelial Cells**; Xinggui Shen¹; Christopher G. Kevil¹; ¹LSU Health-Shreveport, Shreveport, LA
- MP 582 **Phosphoproteomic Evaluation of Chimeric Proteins**; Katelyn Ludwig¹; Nirmalya Sen²; Natasha J Caplen²; Amanda B Hummon¹; ¹University of Notre Dame, Notre Dame, IN; ²NIH, Bethesda, MD
- MP 583 **The Functions of Serine 687 Phosphorylation of Human DNA Polymerase η in UV Damage Tolerance**; Xiaoxia Dai¹; Changjun You¹; Yinsheng Wang¹; ¹UC Riverside, Riverside, CA
- MP 584 **Phosphorylation Dynamics and Interacting Proteins of MAP Kinase 4 Revealed by Proteomics**; Tong Zhang¹; Jacqueline D Schneider²; Craig P. Dufresne³; Alice C Harmon²; sixue chen²; ¹University of Florida, Gainesville, FL; ²University of Florida, Gainesville, Florida; ³Thermo Fisher Scientific, West Palm Beach, FL
- MP 585 **Perturbation of the Phosphoproteome of Colony Stimulating Factor 3 Receptor (CSF3R) in Normal Myeloid Development, Myeloid Leukemia and Neutrophilic Leukemia**; Pankaj Dwivedi¹; David Muench²; Mohammad Azam²; Harry Leighton Grimes²; Kenneth D Greis¹; ¹University of Cincinnati, Cincinnati, OH; ²Cincinnati Children's Hospital Medical Center, Cincinnati, OH
- MP 586 **A Panoramic Survey of Cellular Signaling in Human Gastric Cancer Cells by Monitoring both Phosphotyrosine and Acetyl-Lysine Post-Translational Modifications**; Jeffrey C Silva¹; Cammarata John²; Hamza Ghaith¹; Manor Askenazi¹; Jun Zhu³; Zhongyi Cheng³; ¹Lighthouse Proteomics, Beverly, MA; ²Adeptix Corporation, Beverly, MA; ³PTM BioLab (Hangzhou) Co. Ltd, Hangzhou, China
- MP 587 **Updating and Expanding the PTM Catalog of Acid-Soluble Tau: A Case for Multiplexed Proteomic Analysis**; Gogce Crynen¹; Robert Pelot¹; Craig P Dufresne²; Jon M Reed¹; Prashanthi Vallabhaneni¹; Benoit Mouzon¹; Laila Abdullah¹; James E Evans¹; Fiona Crawford¹; ¹Roskamp Institute, Sarasota, FL; ²Thermo Fisher Scientific, West Palm Beach, FL
- MP 588 **Identification of Cross-Linked Peptides in Proteins Subjected to Photo-Oxidation**; Michele Mariotti¹; Fabian Leinisch²; Diana Julie Oersnes-Leeming³; Michael J Davies²; Birte Svensson⁴; Per Hägglund⁴; ¹Technical University of Denmark, Kongens Lyngby, Denmark; ²University of Copenhagen, Copenhagen, Denmark; ³Nordic Bioscience, Herlev, Denmark; ⁴Technical University of Denmark, Lyngby, Denmark
- MP 589 **msViz, a Zero Learning Curve Graphical Software Tool for Detailed Manual Validation and Quantitation of Post-Translational Modifications**; Manfredo Quadroni¹; Roman Mylonas²; Trinidad Martin Campos^{2,3}; Alexandre Masselot²; Patrice Waridel¹; Ioannis Xenarios²; ¹CIG - University of Lausanne, Lausanne, Switzerland; ²Vital-IT Group - Swiss Institute of Bioinformatics, Lausanne, Switzerland; ³University of Geneva, Geneva, Switzerland

- MP 590 **Sequential Immunoaffinity Purification of Post-Translationally Modified Peptides for Improved Enrichment Specificity**; Matthew P. Stokes¹; Charles L. Farnsworth¹; Jian Min Ren¹; Kimberly A Lee¹; Xiaoying Jia¹; Hongbo Gu¹; Vicky Yang¹; ¹Cell Signaling Technology, Inc. Danvers, MA
- MP 591 **Metabolomics-Assisted Proteomics Reveals the Function of Lysine Succinylation and SIRT5 in Regulation of β -Oxidation of Long-Chain Fatty Acids**; Sushabhan Sadhukhan¹; Xiaojing Liu¹; Ornella D Nelson¹; John A Stupinski²; Sheng Zhang¹; Robert S Weiss¹; Jason W Locasale¹; Hening Lin¹; ¹Cornell University, Ithaca, NY; ²Cornell University, New York, NY
- MP 592 **Mass Spectrometry Based Identification and Characterization Studies of Post Translational Modification Citrullination**; Mandvi Sharma¹; Damagard Dres²; Anne Christian-Bay Jensen³; Claus Nielsen⁴; Birte Svensson⁵; Per Hagglund⁶; ¹PhD, Department of Systems Biology, Denmark Technical University, Copenhagen, Denmark; ²Institute for Inflammation Research, Department of Infectious Diseases and Rheumatology, Copenhagen University Hospital, Rigshospitalet, Copenhagen, Denmark; ³Principal Scientist, Head of Rheumatology, Nordic Biosciences, Copenhagen, Denmark; ⁴Professor, Consultant Physician, Head of Department of Rheumatology, Rigshospitalet, Copenhagen, Denmark; ⁵Professor Enzyme and Protein Chemistry Department of Systems Biology The Technical University of Denmark, Copenhagen, Denmark; ⁶Associate Professor, Department of Systems Biology, Technical University of Denmark, Copenhagen, Denmark
- MP 593 **Characterization of Non-Heme Iron Enzymes Using Mass Spectrometry**; Yi Pu¹; Cheng-Hsuan Wu¹; Deborah R. Leon¹; Pinghua Liu¹; Catherine E. Costello¹; ¹Boston University, Boston, MA
- MP 594 **Evolutionary Conservation of Sirtuin Lipoamidase Activity from Bacteria to Human Mitochondria**; Elizabeth A Rowland¹; Todd M Greco¹; Caroline K Snowden¹; Ileana M. Cristea¹; ¹Princeton University, Princeton, NJ
- MP 595 **Detecting Changes in the Epimerization of Water-Soluble and Water-Insoluble Crystallin Proteins Using Tandem LC-MS**; Yana Lyon¹; ¹Riverside, CA
- MP 596 **Measurement of the Dynamics of Histone Methylation by One-Carbon Metabolic Isotope Labeling and HCD Methylation-Signature-Ions Detection**; Hui Tang¹; KANGLING ZHANG¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX
- MP 597 **Effects of MK-801 and Clozapine on the Proteome of Cultured Human Oligodendrocytes**; Juliana Silva Cassoli¹; Keiko Iwata²; Johann Steiner³; Paul C. Guest¹; Juliana Minardi Nascimento¹; Daniel Martins-de-Souza¹; ¹Laboratory of Neuroproteomics, Department of Biochemistry and Tissue Biology, Institute of Biology, University of Campinas, Campinas, SP, Brazil; ²University of Fukui, Fukui, Japan; ³Department of Psychiatry, University of Magdeburg, Magdeburg, Germany
- MP 598 **Proteomics of Benign and Metastatic Triple Negative Breast Cancer Cells and Cybrids**; Vadhiraja B Bhat¹; Durairaj Renu²; Akanksha Mishra²; Pramila Tata²; Jun Hyoung Park³; Santhosh Kumar³; Sajna A Vithayathil³; Nagireddy Putluri³; Efrosini Tsouko³; Taraka R Donti³; Daniel E Frigo³; Chad J Creighton³; Michael T. Lewis³; Arun Sreekumar³; Lee-Jun Wong³; Benny A Kaiparettu³; ¹Agilent Technologies, Wilmington, DE; ²Strand Life Sciences, Bangalore, India; ³Baylor College of Medicine, Houston, TX
- MP 599 **Targeted Proteomic Analysis of FFPE Bone Metastases from Lung Cancer and Other Malignancies**; Chao Gong¹; Fabiola Cecchi¹; Adele Blackler¹; Wei-Li Liao¹; Marlene Darfler¹; Todd Hembrough¹; ¹NantOmics, Rockville, MD
- MP 600 **Comprehensive Proteome Characterization of Pancreatic Cyst Fluid from Intraductal Papillary Mucinous Neoplasm (IPMN) by LC-MS/MS**; Joonho Park¹; Dohyun Han²; Misol Do³; Mee Joo Kang⁴; Jin-Young Jang⁴; Youngsoo Kim¹; ¹Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; ²Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; ³Department of Biomedical Science, Seoul National University College of Medicine, Seoul, Korea; ⁴Department of Surgery, Seoul National University College of Medicine, Seoul, Korea
- MP 601 **Epitope Identification of Human α -Galactosidase A to a Monoclonal Antibody by Affinity Mass Spectrometry**; Zdenek Kukacka^{1,2}; Marius Iurascu^{1,2}; Yannick Baschung¹; Mary Murphy⁴; Jeff Bornheim⁴; Michael Przybylski^{1,2}; ¹Steinbeis Centre Biopolymer Analysis and Biomedica, Ruesselsheim, Germany; ²University of Konstanz, Konstanz, Germany; ³University of Rostock, Rostock, Germany; ⁴Ametek-Reichert Technologies, Buffalo, NY
- MP 602 **Proteomics Identifies Three New Types of Amyloidosis Associated with Distinctive Clinical Phenotypes**; Surendra Dasari¹; Jason D Theis¹; Julie A Vrana¹; Samih H Nasr¹; Sanjeev Sethi¹; Paul J Kurtin¹; ¹Mayo Clinic, Rochester, MN
- MP 603 **Minimal Residual Disease in Multiple Myeloma by LC-MS/MS by Analysis of Immunoglobulin Heavy and Light Chain CDR Tryptic Peptides**; Linda M Benson¹; Angela Dispenzieri¹; David L. Murray¹; H. Robert Bergen^{III}²; ¹Mayo Clinic, Rochester, MN; ²Mayo Clinic, Rochester, MN
- MP 604 **Pharmacoproteomics Identifies the Drug Efficacy Mechanism in Acamprosate Treatment of Alcoholism**; Caroline M Germany¹; Ashlie N Reker¹; Hyung W Nam¹; ¹LSU Health Science Center, Shreveport, LA
- MP 605 **A Network Based Approach to Understand the Brain Proteome in Alzheimer's Disease**; Nicholas Seyfried¹; Eric B Dammer¹; Vivek Swarup²; Duc Duong¹; Luming Yin¹; Juan C Troncoso³; Madhav Thambisetty⁴; Daniel Geschwind²; James Lah¹; Allan Levey¹; ¹Emory University School of Medicine, Atlanta, GA; ²UCLA, Los Angeles, CA; ³Johns Hopkins University School of Medicine, Baltimore, MD; ⁴National Institutes of Health, Bethesda, MD
- MP 606 **To Pool or Not to Pool: Discovery of Biomarkers for Sjögren's Syndrome Using Mass Spectrometry-Based Proteomics**; Wanlu Qu¹; Driss Zoukhri²; Athena Papas²; Markus Hardt¹; ¹The Forsyth Institute, Cambridge, MA; ²Tufts University, Medford, MA
- MP 607 **Analysis of Monoclonal Immunoglobulins from Multiple Myeloma Patients by Use of 21 Tesla FT-ICR MS/MS**; Lidong He¹; Lissa Anderson²; David R Barnidge³; David L Murray³; Christopher L Hendrickson²; Alan G Marshall¹; ¹Florida State University, Tallahassee, Florida; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Mayo Clinic / DLMP, Rochester, MN
- MP 608 **Understanding the Molecular Mechanisms Underlying Cisplatin Resistance in Ovarian Cancer Cells**; Yi Huo¹; Yuling Chen²; Chongdong Liu³; Zhenyu Zhang³; HAITENG DENG⁴; ¹MOE Key Laboratory of Bioinformatics, Tsinghua University, Beijing, China, 100084, Beijing, China; ²Tsinghua University, Beijing, China; ³Chaoyang Hospital Affiliated to Capital Medical University, Beijing, China; ⁴Tsinghua University, Beijing
- MP 609 **Apolipoprotein Kinetics Measured in Human HDL by HR/AM-PRM Unveils a Novel Picture of HDL Metabolism**; Lang Ho Lee¹; Allison B Andraski²; Brett Pieper¹; Frank M Sacks²; Masanori Aikawa¹; Sasha A Singh¹; ¹Center for Interdisciplinary Cardiovascular Science,

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- Brigham and Women's Hospital and Harvard Medical School, Boston, MA; ²Department of Nutrition, T.H. Chan Public Health School of Harvard University, Boston, MA
- MP 610 **Relevance of Albumin Bound Iron in Ovarian Cancer as Determined by ICP-MS;** Lindsay Schambeau¹; Lauren Amable²; Jana Rucker¹; Michael Finan¹; Rodney Rocconi¹; Lewis Pannell¹; ¹Mitchell Cancer Institute, Mobile, AL; ²National Institutes of Health, Bethesda, MD
- MP 611 **Proteomic Analysis of an ALDH Sub-Population in Colorectal Cancer Identified by Liquid Chromatography-Mass Spectrometry;** Rui Yang¹; Xinhua Liu²; Smathorn Thakolwiboon³; Jianhui Zhu¹; Xiucong Pei¹; Zhijing Tan¹; Mingrui An¹; Jun Cao¹; Jing Wu¹; David M Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²Shanghai University, Shanghai, CHINA; ³Mahidol University, Bangkok, Thailand
- MP 612 **Ion Current-based Proteomic Profiling in Understanding the Mechanism of Tumor Necrosis Factor Alpha on Myogenic Differentiation;** Chengjian Tu¹; Jun Li²; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²University at Buffalo SUNY, Williamsville, NY
- MP 613 **Characterization of O- and N-Glycosylations of Immunoglobulin A in IgA Nephropathy;** Jean-Marie Schmitter¹; Katell Bathany²; Christelle Oblet³; Jean-Claude Aldigier³; Anne Druilhe³; ¹University of Bordeaux, Bordeaux, France; ²University of Bordeaux, Bordeaux, France; ³University of Limoges, Limoges, France
- MP 614 **Effect of Radiotherapy on Protein Levels in Blood Plasma Collected from Breast Cancer Patients;** Catherine C Going¹; Marta Vilalta¹; Marjan Rafat¹; Melissa Jenkins¹; Kathleen C Horst¹; Edward E Graves¹; Sharon J Pitteri¹; ¹Stanford University School of Medicine, Palo Alto, CA
- MP 615 **Prions in Hormonal Replacement Therapy?;** Tanja Panic-Jankovic¹; Maria Zellner²; Goran Mitulovic²; ¹Medizinische Universitaet Wien, Vienna, Austria; ²Medical University of Vienna, Vienna, Austria
- MP 616 **Mass Spectrometry Based Proteomic Investigation of Annulus Fibrosus and Nucleus Pulposus of the Mature Bovine Intervertebral Disc;** Willem Duckworth¹; Ashley Brisbin¹; Kelly L Wormwood¹; Emmalyn J Dupree¹; Jessica Roberge¹; Devika Channaveerappa¹; Petra Kraus¹; Thomas Lufkin¹; Costel C Darie¹; ¹Clarkson University, Potsdam, NY
- MP 617 **Single Amino Acid Variation Profiles of the MCF7 Breast Cancer Cell Line Using LC-MS/MS;** Zhijing Tan¹; Song Nie^{1,2}; Mingrui An¹; Rui Yang¹; Jun Cao¹; Xiucong Pei¹; David M. Lubman¹; ¹The University of Michigan, Ann Arbor, MI; ²Pacific Northwest National Laboratory, Richland, WA
- MP 618 **Evaluation of Undifferentiated State of Human iPS Cells by Non-Invasive LC-MS/MS Analysis Approach Using Cell Culture Supernatant as Samples;** Takashi Suzuki¹; Gamo Kentaro²; Hatabayashi Kunitada²; Takahashi Masatoshi¹; Kagawa Kenichi²; Ogura Tairo³; Hiramaru Daisuke¹; Toyoda Kenichi¹; Ozaki Shigenori²; ¹Shimadzu Corporation, Kyoto, Japan; ²Tokyo Electron Limited, Kobe, Japan; ³Shimadzu Scientific Instruments, Inc. Columbia
- MP 619 **Quantitative Proteomics Analysis Reveals Molecular Signatures Associate with LPS, Betamethasone, and Magnesium Sulfate Treatment in E15 Murine Gastrointestinal Tract;** Elizabeth Yohannes¹; Jessica L. Slack¹; Vivek Ramachandran¹; Andrew S. Thagard²; Mark Wingerd¹; Avedis Kazanjian¹; ¹Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, Washington; ²Maternal Fetal Medicine, Madigan Army Medical Center, Tacoma, Washington
- MP 620 **Proteomics of Globo H High/Low BxPC-3 Pancreatic Cancer Cell Line;** Sheng-Ta Tsai¹; Hsin-Ying Han¹; Shok-Li Ng¹; Chia-Ning Shen¹; Chung-Hsuan Chen¹; ¹Genomics Research Center, Academia Sinica Taipei, Taiwan
- MP 621 **Proteomic Analysis by SILAC to Distinguish between Salmonella Lipopolysaccharide (LPS) and Monosodium Urate (MSU) Crystals Induced Inflammation in Macrophages;** Sarbjee Makkar¹; Rohana Liyanage¹; Jr Jackson O Lay¹; ¹University of Arkansas, Fayetteville, AR
- PROTEOMICS: QUANTITATIVE**
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- MP 622 **Quantitation of Immunoglobulin Alpha from Whole Gut Lavage Fluid Using the Thermo Q-Exactive Plus;** Joseph Otto¹; Crystal Daniels¹; Lindsay Schambeau¹; Jana Rucker¹; ¹Mitchell Cancer Institute, Mobile, AL
- MP 623 **Targeted Quantitation of Crbpl in Cancer Cells through a Bottom-Up Approach;** Wenjing Li¹; Jianshi Yu¹; Claire Louise Carter¹; Jace W Jones¹; Maureen A Kane¹; ¹University of Maryland School of Pharmacy, Baltimore, MD
- MP 624 **Kinase Activity Profiling of Lung Adenocarcinoma to Understand Cancer Signaling and Select Targeted Therapeutics;** Melissa A. Hoffman^{1,2}; Bin Fang¹; Stephen Brantley¹; Fumi Kinose¹; Eric Welsh¹; Steven A. Eschrich¹; Eric B. Haura¹; John M. Koomen¹; ¹Moffitt Cancer Center, Tampa, FL; ²University of South Florida, Tampa, FL
- MP 625 **Label-Free Quantitative Proteomics Profiling of Human Osteoclast Activation, Differentiation and anti-TNF Biologics Treatment;** Chenqi Hu¹; Bohdan Harvey¹; Zehra Kaymakalan¹; Edit Tarcsa¹; Dongdong Wang¹; Yu Tian¹; ¹Abbvie Bioresearch Center, Worcester, MA
- MP 626 **Protein Biomarker Quantitation from Human Blood and Plasma Using Novel Collection Technology by LCMS/MS;** Alan Barnes¹; Neil Loftus²; Jérôme Vialaret³; Christophe Hirtz³; Sylvain Lehmann³; ¹Shimadzu MS/BU, Manchester, Greater Manchester; ²Shimadzu, Manchester, UK; ³CHU de Montpellier, Montpellier, France
- MP 627 **In Depth Quantification of Extracellular Matrix Proteins from Human Pancreas for Tissue Engineering;** Fengfei Ma¹; Christopher Lietz²; Sara Sackett³; Dan Tremmel³; Jon Odorico³; Lingjun Li^{1,2}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ³Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- MP 628 **Identification of Interaction Networks of Mutant and Wild-Type IDH1 in Glioma Cell Lines;** Nina Overbeck¹; Anja Stefanski¹; Vanessa Scherbaum²; Christiane Knobbe-Thomsen²; Kai Stühler¹; ¹Molecular Proteomics Laboratory, Heinrich-Heine-University, Düsseldorf, Germany; ²Department of Neuropathology, Heinrich-Heine-University, Düsseldorf, Germany
- MP 629 **Quantitative MRM Assays of Salivary Proteins for Biomarker Assessment Studies;** Andrew J Percy¹; Darryl B Hardie¹; Juncong Yang¹; Armando Jardim²; Yassene Mohammed^{1,3}; Monica H. Elliott¹; Christoph H. Borchers⁴; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Institute of Parasitology, McGill University, Montreal, QC, Canada; ³Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; ⁴University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 630 **Toward the Development of a Scheduled GeLC-MRM Method for High-Throughput Quantitative Profiling of Small GTPases in Cancer Cells;** Ming Huang¹; Yinsheng Wang²; ¹University of California, Riverside, Riverside, California; ²University of California, Riverside, Riverside, CA
- MP 631 **Targeted Proteomic Analysis Using Parallel Reaction**

- Monitoring Revealed Longitudinal Change in Level of Proteins in Activation of BV2 Mouse Microglia;** Woo Jongmin¹; Han Dohyun^{2,3}; Kim Youngsoo²; ¹Department of Biomedical Sciences, Seoul National University, College of Medicine, Seoul, Korea; ²Department of Biomedical Engineering, Seoul National University, College of Medicine, Seoul, Korea; ³Biomedical Research Institute, SNUH, Seoul, Korea
- MP 632 **Changes in Lipid Raft Proteome upon TNF- α Stimulation of Cystic Fibrosis Cells Using SILAC;** Cerina Chhuon¹; Iwona Pranke²; Florence Borot²; Danielle Tondelier²; Joanna Lipecka³; Janine Fritsch²; Marc Chanson⁴; Aleksander Edelman²; Mario Ollero⁵; Chiara Ida Guerrero¹; ¹Proteomic Platform Necker, PPN-3P5, Structure Fédérative de Recherche SFR Necker US24, 75015, Paris, France; ²Institut Necker Enfants Malades, INSERM, U1151, Paris, France; ³The CPN Proteomics Facility – 3P5, Center of Psychiatry and Neuroscience, UMR INSERM 894, 75014, Paris, France; ⁴Geneva University Hospitals and University of Geneva, 1211, Geneva, Switzerland; ⁵Institut Mondor de Recherche Biomédicale, INSERM, U955, and Université Paris Est Créteil, 94010, Créteil, France
- MP 633 **MRM Quantitation of an In-depth Panel of Candidate Disease-linked Proteins in Various Mouse Tissues;** Sarah Michaud¹; Andrew Percy²; Nicholas Sinclair²; André LeBlanc²; Suping Zhang³; Christoph H. Borchers^{2,4}; ¹MRM Proteomics Inc, Victoria, BC, Canada; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ³MRM Proteomics, Inc., Victoria, BC, Canada; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 634 **The Proteomic Landscape of Breast Patient-Derived Xenografts Reveals Tumor-Specific Education of the Cancer Microenvironment;** Xuya Wang¹; Petra Erdmann-Gilmore²; Rosa Viner³; Matthew R Meyer²; Timothy J Stuhlmiller⁴; Sherri R Davies²; Shunqiang Li²; Qiang Zhang²; Arshag D Mooradian²; Kuan-lin Huang⁵; Ryan Bomgarden⁶; Li Ding⁵; Matthew J Ellis⁷; John C Rogers⁶; Gary L Johnson⁴; Reid R Townsend²; David Fenyö⁸; Jason M Held^{2,8}; ¹NYU School of Medicine, New York City, NY; ²Washington University School of Medicine, Saint Louis, MO; ³Thermo Fisher Scientific, San Jose, CA; ⁴Department of Pharmacology University of North Carolina, Chapel Hill, NC; ⁵The Genome Institute Washington University, Saint Louis, MO; ⁶Thermo Fisher Scientific, Rockford, IL; ⁷Baylor College of Medicine, Houston, TX; ⁸Department of Anesthesiology Washington University, Saint Louis, MO
- MP 635 **The Pathway Activity of Fatty Acid β -Oxidation is Up-Regulated in the Skeletal Muscle Mitochondria of T2DM Mouse Model;** Zhou Yang^{1,2}; Hou Guixue^{1,3}; Wu Lin¹; Lou Xiaomin¹; Ren Yan²; Su Siyuan^{1,2}; Deng Yamei^{1,2}; Li Qidan^{1,2}; Zhang Yue^{1,2}; Zi Jin²; Liu Siqi^{1,2}; ¹CAS Key Laboratory of Genome Sciences and Information, Beijing Institute of Genomics, Chinese Academic of Sciences, Beijing, China; ²BIG-Shenzhen, Shenzhen, China; ³BGI shenzhen, Shenzhen, China
- MP 636 **In-Depth Quantitative Proteomic Analysis of Human Breast Cancer Cells in Response to Nicotinamide;** Dohyun Han^{1,2}; Ji Young Kim³; Joonho Park²; Han Suk Ryu³; ¹Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; ²Department of Biomedical Engineering, Seoul National University Hospital, Seoul, Korea; ³Department of Pathology, Seoul National University Hospital, Seoul, Korea
- MP 637 **iTRAQ Based Quantitative Proteomics of a Brain-Enriched Cytosolic Protein Fraction in Schizophrenia;** Erika Velásquez¹; Daniel Martins-de-Souza²; Ingrid Velásquez³; Andrea Schmitt⁴; Fabio Cs Nogueira⁵; Gilberto B Domont¹; ¹Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; ²Unicamp, Campinas, SP; ³University of Carabobo, Valencia, Venezuela; ⁴Ludwig Maximilian University of Munich, Munich, Germany; ⁵UFRJ, Rio de Janeiro, Rio de Janeiro
- MP 638 **Challenges of Using Isobaric Labeling for In-Depth Analysis of Large Numbers of Plasma Samples in a Cardiotoxicity Biomarker Discovery Study;** Pengyuan Liu¹; Lynn A. Beer¹; Bonnie Ky²; David W Speicher¹; ¹The Wistar Institute, Philadelphia, PA; ²University of Pennsylvania, Philadelphia, PA
- MP 639 **Quantitative Multiplexed Isobaric Tag-Based Proteomic and Phosphoproteomic Profiling Reveals Nicotine and Cigarette Smoke Extract-Induced Alterations in Human Pancreatic Stellate Cells;** Joao A Paulo¹; Steven P Gygi²; ¹Harvard, Boston, MA; ²Harvard Medical School, Boston, MA
- MP 640 **SILAC-based Phosphoproteomic Analysis of PTH1R Signaling in Proliferating Osteoblasts;** Lauren E Ball¹; Grace Williams¹; Jennifer Bethard¹; Louis Luttrell¹; ¹Medical Univ of S Carolina, Charleston, SC
- MP 641 **Quantitative Temporal Proteomics of Flow Cytometry Isolated Virus-Driven MDSCs;** Derek Clements¹; Patrick Murphy²; Youra Kim¹; Andra Sterea³; Shekoufeh Almasi³; Namit Holay¹; Prathyusha Konda²; Joao Paulo⁴; Steven P Gygi⁴; Shashi Gujar²; Patrick Lee^{1,2}; ¹Department of Pathology, Dalhousie University, Halifax, NS, Canada; ²Department of Microbiology & Immunology, Dalhousie University, Halifax, NS, Canada; ³Department of Biology, Dalhousie University, Halifax, NS, Canada; ⁴Harvard University, Boston
- MP 642 **Down Regulation of Glycolysis Pathway in PICALM Depleted Cells;** Barsam Mirfatah¹; Hui Tang¹; Cheryl F Licht¹; Fernanda Laezza¹; Kangling Zhang¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX
- MP 643 **Phosphoproteomic and Glycoproteomic Studies of Tonic and Activated B Cell Receptor Signaling in Burkitt's Lymphoma;** Jasmin Corso¹; Kuan-Ting Pan¹; Roland Walter²; Carmen Döbele²; Sebastian Mohr²; Christof Lenz^{1,3}; Hubert Serve^{2,4}; Henning Urlaub^{1,3}; Thomas Oellerich^{2,4,5}; ¹Bioanal. MS Group, Max Plank Inst for Biophys Chem, Goettingen, Germany; ²Department of Hematology/Oncology, Johann Wolfgang Goethe University, Frankfurt, Germany; ³Bioanalytics, University Medical Center Göttingen, Institute for Clinical Chemistry, Goettingen, Germany; ⁴German Cancer Consortium/ German Cancer Research Center, Heidelberg, Germany; ⁵Department of Haematology, University of Cambridge, Cambridge, United Kingdom
- MP 644 **Quantitative Profiling of Peroxisome Proliferation in the Heart by Selected Reaction and Selected Ion Monitoring. Effects of High Fat Diets;** Caroline Kinter¹; Maria Thomas¹; David Gutierrez¹; Szweda Luke¹; Michael Kinter¹; ¹Oklahoma Medical Research Foundation, Oklahoma City, OK
- MP 645 **MS1-Based Quantitative Proteomics Investigation of Mechanisms Underlying Gemcitabine and Trabectedin Synergism with High Multiplexing Capacity and Extremely Low Missing Value;** Shichen Shen¹; Xin Miao¹; Jun Li¹; Xiaomeng Shen¹; Xue Wang¹; William Jusko¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY
- MP 646 **Understanding Proteomic Alterations in GBM Tumors Associated with the Subventricular Zone: a Quest for Better Prognosis;** Ghantasala Saicharan¹; Gollapalli Kishore²; Shailendra Rane³; Deepthi Bhandarkar³; Sanjeeva Srivastava²; Aliasgar Moiyadi⁴; ¹Indian Institute of Technology, Bombay, Mumbai, India; ²Indian Institute of Technology, Bombay, Mumbai, India; ³Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA; ⁴Tata Memorial Centre's-Advanced Centre for Research, Training and Education in Cancer, Kharghar, Navi Mumbai, India

- MP 647 **Exploration of Novel Mechanisms for Synergy of Paclitaxel and Birinapant through Large-scale Quantitative Label-free LC/MS Proteomics**; Xue Wang¹; Jin niu¹; Jun Li²; Shichen Shen²; Xiaomeng Shen²; Jun Qu²; ¹University at Buffalo, Buffalo, NY; ²Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY
- MP 648 **ProteOMZ: Development of Biogeochemically Relevant Peptide Biomarkers for High-Throughput Marine Microbial Ecosystem Characterization in Oceanic Oxygen Minimum Zones**; Mak Saito¹; Matt McIlvin¹; Dawn Moran¹; Alyson Santoro²; Chris Dupont³; Michael Rappe⁴; ¹Woods Hole Oceanographic Institution, Woods Hole, MA; ²University of Maryland Horn Point Laboratory, Cambridge, MD; ³J.C. Venter Institute, La Jolla, CA; ⁴Hawaii Institute of Marine Biology, University of Hawaii, Manoa, HI
- MP 649 **Sensitive, Fast and Robust Quantification of Antibodies in Complex Matrices by Capillary Flow UHPLC and High Resolution Accurate Mass MS**; Alexander Boychenko¹; Stephan Meding²; Martin Samonig²; Remco Swart²; ¹Thermo Fisher Scientific, Bremen, DE; ²Thermo Fisher Scientific, Germering, DE
- MP 650 **Src-Family Kinase Signaling Mediating Gemcitabine Resistance in Gall Bladder Cancer Revealed by Quantitative Phosphoproteomics**; Patricia García¹; Jun Zhong²; Carolina Bizama¹; Jaime Espinoza¹; Juan Carlos Roa¹; Pamela Leal³; ¹Department of Pathology, School of Medicine; Center for Investigation in Translational Oncology (CITO), FONDAP-ACCDIS, Pontificia Universidad Católica de Chile, Santiago, Chile; ²Delta Omics Biotechnology, Catonsville, MD; ³Center of Genetic and Immunological Studies (CEGIN) and Scientific and Technological Bioresource Nucleus (BIOREN). Universidad de La Frontera, Temuco, Chile
- SMALL MOLECULES: QUALITATIVE ANALYSIS**
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- MP 651 **Identification of Chemical Ingredients from *Ginkgo biloba* Extract Using UHPLC-QTOF/MS Coupled with PCDL Library**; Guoqiang Liu¹; Shan-An Chan²; ¹Agilent Technology, Inc. Shanghai, China; ²Agilent Technology, Inc. Taipei Taiwan, Taiwan
- MP 652 **Collision-Induced Dissociation MS/MS of Cimitrypazepines, A New Class of Alkaloids from Black Cohosh (*Actaea racemosa*)**; Dejan Nikolic¹; David C Lankin¹; Richard van Breemen¹; ¹University of Illinois College of Pharmacy, Chicago, IL
- MP 653 **Dereplication of Fungal Secondary Metabolites by UPLC-PDA-HRMS-MS/MS and Mass Defect Filtering**; Noemi Paguigan¹; Tamam M. El-Elmat^{1,2}; Diana Kao^{1,2}; Huzefa A. Raja¹; Cedric J. Pearce³; Nicholas H Oberlies¹; ¹Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; ²Chemistry and Biochemistry Department, Greensboro, NC; ³Mycosynthetix, Inc., Hillsborough, NC
- MP 654 **Development and Evaluation of a Dual Separation, High-Resolution, nano-ESI-LC-MS/MS Approach for Dissolved Soil Organic Matter Characterization**; Mallory P Ladd^{1,2}; Robert Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee-Knoxville, Knoxville, TN
- MP 655 **Formation of m/z 92 Ion During Fragmentation of Deprotonated N-butyl Benzenesulfonamide**; Chongming Liu¹; Athula B. Attygalle¹; ¹Stevens Institute of Technology, Hoboken, NJ
- MP 656 **Gas-phase Methylation of Benzene by an Internal Electrophilic Aromatic Addition Mechanism Mediated by *in-situ* Generated Methylcarbenium Ion**; Hanxue Xia¹; Athula Attygalle²; Yong Zhang²; ¹SIT, Jersey city, New Jersey; ²Stevens Institute of Technology, Hoboken, NJ
- MP 657 **Non-Targeted Screening of Tattoo Ink Contaminants Using Liquid Chromatography/ High-Resolution Mass Spectrometry and Chemometrics**; Caitlin N. Kneapler¹; Ann M. Knolhoff¹; Clark Ridge¹; Fred Fry¹; Timothy R Croley¹; ¹FDA/CFSAN, College Park, MD
- MP 658 **Applications of Infrared Ion Spectroscopy in Bioanalytical Chemistry**; Jonathan Martens¹; Giel Berden¹; Jos Oomens¹; ¹FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands
- MP 659 **A Bayesian Prior Probability Model to Improve the Confidence of Chemical Identification**; Tyler A. Zimmerman¹; W.Gary Mallard²; Tytus D Mak²; Nirina Rabe Andriamaharavo²; Dmitrii V Tchekhovskoi²; Stephen E Stein²; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²National Institute of Standards & Technology, Rockville, MD
- MP 660 **Investigation of the Metabolites of the HIF-Stabilizer FG-4592, Formed by Four *in vitro* Models, Using High Resolution Mass Spectrometry**; Annelie Hansson¹; Mario Thevis²; Geoff Miller³; Daniel Eichner³; Ulf Bondesson¹; ¹Mikael Hedeland^{1,4}; ¹Uppsala University, Uppsala, SE; ²German Sport University, Cologne, DE; ³Sports Medicine Research and Testing Laboratory, Salt Lake City, UT; ⁴National Veterinary Institute, Uppsala, SE
- MP 661 **The ETD-Like Fragmentation for Small Molecules**; Romain Huguet¹; Chad R Weisbrod¹; Mark Berhow²; Vlad Zabrouskov¹; Jae Schwartz¹; Tim J Stratton¹; ¹Thermo Fisher Scientific, San Jose, CA; ²USDA, ARS NCAUR Peoria, IL
- MP 662 **Application of TOF MS instrument in Bioanalysis – A Case Study**; Shaokun Pang¹; Weixing Sun²; Adrien Musuku²; Xavier Misonne³; ¹SCIEX, Redwood City, CA; ²Pharmascience, Montreal, Canada; ³SCIEX, Lorraine, QC
- MP 663 **On-Line Chiral Analysis of Reaction Mixtures Using the Kinetic Method**; Ryan M Bain¹; Xin Yan¹; Shannon A Raab¹; Stephen T Ayrton¹; Tawnya G Flick²; Graham R Cooks¹; ¹Purdue University, West Lafayette, IN; ²Amgen, Inc., Thousand Oaks, CA
- MP 664 **Automated Correlation between Structural Isomers and Fragment Ion Spectra Using a Novel Fragmentation Prediction Engine**; Kirsten Hobby¹; Richard T Gallagher²; ¹Shimadzu MS/BU, Manchester, Lancashire; ²AstraZeneca, Macclesfield, UK
- MP 665 **Effects of Low Percentage Non-Ionic Additives on Charge State and Ion Intensity in Electrospray Ionization for Small Molecule Analysis**; Jeffrey Alberts¹; Kenneth J Ruterbories¹; David W Bedwell¹; Kishore K Katayan¹; Kenneth C Cassidy¹; ¹Eli Lilly and Company, Indianapolis, IN
- MP 666 **Understanding Paper Degradation: Identification of Products of Cellulosic Paper Decomposition at the Wet-Dry “Tideline” Interface Using GC-MS and LTQ Orbitrap**; Sergey Sladkevich¹; Anne-Laurence Dupont²; Michel Sablier²; Richard B. Cole¹; ¹Sorbonne Universités, UPMC Univ Paris 06, Paris, France; ²Muséum National d'Histoire Naturelle, Paris, France
- MP 667 **Development of a GC-MS Method for Structure Elucidation of Disubstituted Naphthalenes**; Kirill Tretyakov¹; Stephen Stein¹; Anzor Mikaia¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- MP 668 **Substituting Atmospheric Solid Analysis Probe Ionization for Direct Probe Electron Impact Ionization for Analysis of Alcohols and Hydrocarbons**; Martha M. Vestling¹; Trevor C. Christenson; Stephanie N. Knezz; ¹University of Wisconsin, Madison, WI
- MP 669 **Dosing Syringe Extractables Analysis Using Bench-top Orbitrap Mass Spectrometer**; Kenneth Wong¹; Dujuan Lu¹; Kate Comstock²; ¹SGS, Fairfield, NJ; ²Thermo Fisher Scientific, San Jose, CA

- MP 670 **Identification and Quantitation of IV Bag Extractables Using LC-HRMS and GCMS**; Dujuan Lu¹; Kenneth Wong¹; Kate Comstock²; ¹SGS, Fairfield, NJ; ²Thermo Fisher Scientific, San Jose, CA
- MP 671 **Impurity Profiling of Pharmaceuticals Using a UPLC-ToF Data Independent Acquisition Strategy and Scientific Data and Library Information Systems**; Jayne Kirk¹; Russell Mortishire-Smith¹; Sean McCarthy²; Mark Wrona²; ¹Waters Corporation, Wilmslow, UK; ²Waters Corporation, Milford, MA
- MP 672 **The Application of Electrochemistry/MS to Pharmaceutical Stability Testing and Degradant Synthesis**; Martin Eysberg¹; Jean-Pierre Chervet²; Nico Reinhoud²; Mark Taylor³; Susana da Silva Torres³; ¹Antec LLC, Boston, MA; ²Antec, Zoeterwoude, The Netherlands; ³Pfizer Worldwide Research and Development, Kent, United Kingdom
- MP 673 **Differentiating between Leachates and Process Related Compounds in Drug Substance Using Accurate Mass LC-MS and LC-MS/MS**; George L Perkins¹; Lorraine Hill¹; Gary Campbell¹; Matthew Balmer¹; ¹Sanofi Pasteur Inc, Swiftwater, PA
- MP 674 **Analysis of Celastrol in Rat Brain Tissue and Plasma Samples Using TSQ Quantum Access MAX**; Usha Mishra; Minnmass(Minnesota Mass Spec), Minneapolis, MN
- MP 675 **Determination of Limaprost, an Analogue of PGE1 in Human Plasma by QTRAP® 6500+ and SelexION® Technology**; Gangyi Liu¹; Chao Zhang²; Wenhui Jin³; ¹Xuhui Center Hospital, Shanghai, China; ²SCIEX Asia Pacific Application Support Center, Beijing, China; ³SCIEX Asia Pacific Application Support Center, Shanghai, China
- MP 676 **Effects of Temperature and Anticoagulant on the Stability of Tetracyclines in Whole Blood: Drug-Matrix Equilibrium**; Vinicio Vasquez¹; Richard Lavallée¹; Nikolay I Youhnovski¹; Milton Furtado¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- MP 677 **Extremely Low LC-MS/MS Lithium Adduct Detection of Rapamycin in Animal Blood and Tissues**; Alexandre Pimenov¹; Timothy Samuels¹; ¹Charles River Bioanalysis, Senneville, Canada
- MP 678 **Analyzing Zn-BDPA Probes to Detect Apoptotic Cells in Three-Dimensional Cell Culture System via Mass Spectrometry**; Jessica K Lukowski¹; Eric M Weaver¹; Kasey Clear¹; Bradley D Smith¹; Amanda B Hummon¹; ¹University of Notre Dame, Notre Dame, Indiana
- MP 679 **LC-MS Based Approach to Characterize Non-Specific Binding Inhibitors to Mycobacterium tuberculosis Shikimate Kinase (MtSK)**; Mansour Alturki¹; Madison Jarrard¹; Rene Ngouli¹; Douglas Goodwin¹; Angela Calderon¹; ¹Auburn University, Auburn, AL
- MP 680 **Synthesis and Characterization of Tetrphenylporphyrinate Manganese(III) Siloxides by Silyl Group Transfer from Silanethiols**; Zachary J Tonzetich¹; Daniel J Meiningner¹; Zieph Kasrawi¹; Hadi D Arman¹; Wendell P. Griffith¹; ¹University of Texas at San Antonio, San Antonio, TX

SYSTEMS BIOLOGY (MULTIOMICS AND OTHER)

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- MP 681 **Trans-omics Analysis of Yeast Central Carbon Metabolism by Integration of Metabolome, Proteome and Fluxome Data**; Fumio Matsuda¹; Syunsuke Nishino²; Tairo Ogura³; Atsumi Tomita²; Ichiro Hirano³; Hiroshi Shimizu²; ¹Osaka University, Osaka, Japan; ²Osaka University, Osaka, Japan; ³Shimadzu Corporation, Kyoto, Japan
- MP 682 **Proteomics and Metabolomics Demonstrate Inheritance of Key Energy Pathways in Red Blood Cells**; Erin M. Weisenhorn¹; Thomas J. van't Erve²; Michael S Westphall³; Thomas J. Raife⁴; Joshua J Coon⁵; ¹Integrated Program in

Biochemistry, University of Wisconsin-Madison, Madison, WI; ²Immunity, Inflammation and Disease Laboratory, National Institute of Environmental Health Sciences, Research Triangle Park, NC; ³University of Wisconsin-Madison Genome Center of Wisconsin, University of Wisconsin, Madison, Madison, WI; ⁴Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; ⁵Departments of Chemistry and Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI

- MP 683 **Proteomic and Metabolomic Comparative Analyses of Plasma and Vasculture Tissue from TiO2nanoparticle Exposed Rats**; Megan M. Maurer¹; Jinghai Yi¹; Carroll McBride¹; Timothy R. Nurkiewicz¹; Stephen J Valentine¹; ¹West Virginia University, Morgantown, WV
- MP 684 **Combined Metabolomics-Proteomic Profiling Reveals Intermittent Hypoxia to Result in Lower Productivity on Scale-Up to a 5000-Liter Industrial CHO Bioprocess**; Yuanwei Gao¹; Somak Ray¹; Shujia Dai¹; Alexander R. Ivanov¹; Nicholas R. Abu-Absi²; Amanda M. Lewis²; Zhuangrong Huang²; Xing Zizhou²; Michael C. Borys²; Zheng Jian Li²; Barry L Karger¹; ¹Northeastern University, Boston, Massachusetts; ²Bristol-Myers Squibb, Devens, MA
- MP 685 **Triomics Analysis from Cancer Cells and Tumors: Modeling the Biology of Disease through The Integration of Metabolomics, Lipidomics and Phosphoproteomics**; Susanne Breikopf¹; Min Yuan¹; Ying Xu¹; John M Asara^{1,2}; ¹Beth Israel Deaconess Medical Center, Boston, MA; ²Harvard Medical School, Boston, MA
- MP 686 **Integrated Multi-Omic Analysis of Chinese Hamster Ovary Cells**; Joseph Longworth¹; Javier Gonzalez¹; Paul Dobson²; Josselin Noirel³; Neil Lawrence¹; Mark Dickman¹; David James¹; ¹The University of Sheffield, Sheffield, United Kingdom; ²The University of Manchester, Manchester, United Kingdom; ³Conservatoire National des Arts et Métiers, Paris, France
- MP 687 **Systematic Integration of Multiple 'Omics Data for Yeast Strains Isolated from Different Environments**; Rohith Srivas¹; Barbara Dunn¹; Andreas Huhmer²; Daniel Lopez Ferrer³; Michael Snyder¹; ¹Dept. of Genetics, Stanford University, Palo Alto, CA - California; ²Thermo Fisher Scientific, San Jose, CA; ³ThermoFisher, Palo Alto, CA
- MP 688 **Integrative Analysis of Proteome, Transcriptome, and MHC Class I Ligandome of Human Cancer Cell Lines**; Pedro Navarro¹; Sebastian Boegel²; Jennifer Hahlbrock¹; John C Castle³; Meike Wagner²; Hansjörg Schild¹; Ugur Sahin²; Stefan Tenzer¹; ¹Institute for Immunology, JG University Medical Center, Mainz, Germany; ²TRON – Translational Oncology at the University Medical Center of Johannes Gutenberg University, Mainz, Germany; ³Agenus, 4-Antibody AG, Basel, Switzerland
- MP 689 **Differential Dynamics of the Mammalian mRNA and Protein Expression Response to Misfolding Stress**; Zhe Cheng¹; Guoshou Teo²; Sabrina Krueger³; Tara Rock¹; Hiromi Koh²; Hyungwon Choi²; Christine Vogel¹; ¹New York University, New York, NY; ²National University of Singapore, Singapore, Singapore; ³Max-Delbruck-Center, Berlin, Germany
- MP 690 **High Resolution Mass Spectrometry-Based Subcellular Proteomics of a Human Cell Line**; Aikaterini Geladaki¹; Claire Mulvey¹; Jake Beech¹; Kathryn S Lilley¹; ¹Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom
- MP 691 **A Multi-Molecular Omics Approach to Study Metabolic Shifts in Caveolin-3 Transgenic Mice**; Cristina Coman¹; Denisa Gabriela Hathazi¹; Andreas Roos¹; Robert Ahrends¹; ¹Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany



- MP 692 **Integration of Metabolomic and Proteomic Profiles with Physiological Measures to Understand the Complex Mechanisms of Sodium Fluoroacetate Toxicity;** Nadja Grobe^{1,2}; Meghan K Makley^{2,3}; Mitchell L Meade²; Andrea Hoffmann^{2,3}; Jeffery M Gearhart^{2,3}; ¹The Henry M. Jackson Foundation for the Advancement of Military Medicine (HJF), Wright-Patterson AFB, OH; ²Molecular Bioeffects Branch, Bioeffects Division, Human Effectiveness Directorate, 711th Human Performance Wing, Air Force Research Laboratory, Wright-Patterson AFB, OH; ³The Henry M. Jackson Foundation for the Advancement of Military Medicine (HJF), Wright-Patterson AFB, OH
- MP 693 **In-Depth Secretome Analysis of Ovarian Clear Cell Carcinoma with ARID1A Knockdown and EZH2 Inhibition.;** Aaron R Goldman¹; Benjamin G Bitler¹; Rugang Zhang¹; David W Speicher¹; ¹The Wistar Institute, Philadelphia, PA
- MP 694 **Data-independent Mass Spectrometry: An Effective Tool in Mechanistic Neurotoxicological Research;** Pallavi P Pilaka¹; Pretal P Muldoon¹; Pavel N Lzhnyak¹; Andrew K Ottens¹; ¹Department of Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA
- MP 695 **Data-Driven Construction of Global Drug Mechanisms Enabled by an Integrated High-Throughput Multi-Omics Platform;** Jeremy L Norris¹; Melissa A Farrow¹; Danielle Gutierrez¹; Nicole Muszynski¹; Lauren D Palmer¹; Stacy D Sherrod¹; James C Pino¹; Jamie L Allen¹; Jeffrey M Spraggins¹; Alex Lubbock¹; Ashley T Jordan¹; William J Burns¹; James C Poland¹; Carrie E Romer¹; Nathaniel Braman¹; Yuan-wei Nei¹; Kristie L Rose¹; Salisha Hill¹; Lisa M Manier¹; Tina Tsui¹; M. Ray Keller¹; Stacey A Rutherford¹; Nichole A Lobdell¹; Carlos Lopez¹; D. Borden Lacy¹; John A McLean¹; John P Wikswol¹; Eric P Skaar¹; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN
- MP 696 **Applying Sequence Clustering to Facilitate Sample Comparisons in Metaproteomes Searched Against Different Metagenomes in Human Microbiome Research;** Jose Alfredo Blakeley-Ruiz¹; Weili Xiong²; Yang Song³; Claire Fraser-Liggett³; Robert Hettich²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³University of Maryland Baltimore, Baltimore, USA
- MP 697 **Rapid Changes in the Proteome of Gut Microbiota in Response to Short-Term Dietary Challenges in Baboons;** Prahlad K Rao¹; Kimberly D Spradling-Reeves¹; Vicki Mattern¹; Laura Cox¹; Anthony G Comuzzie¹; Michael Olivier¹; ¹Texas Biomedical Research Institute, San Antonio, TX
- MP 698 **Mass Spectrometry Based Systems Biology Approaches to Understand Platelet Metabolism;** Ottar Rolfsson^{1,2}; Steinn Guðmundsson^{1,2}; Manuela Magnúsdóttir^{1,2}; Freyr Johansson^{1,2}; Ólafur Eysteinn Sigurjónsson^{3,4}; Bernard O Palsson^{1,2}; ¹Center For Systems Biology, Reykjavik, Iceland; ²University of Iceland, Reykjavik, Iceland; ³Reykjavik University, Reykjavik, Iceland; ⁴The Icelandic Blood Bank, Reykjavik, Iceland
- MP 699 **Exercise-Induced Protein Secretion from Muscle;** You Zhou¹; Ji Li¹; Sammy Pardo¹; Dana Mollere¹; Caleb Emmons²; Susan T Weintraub¹; Nicolas Musi¹; ¹Univ. of Texas HSC, San Antonio, TX; ²Proteome Software, Portland, OR
- MP 700 **Data-independent Quantitative Mass Spectrometry in Brain Injury Therapeutic Development;** Pavel Lzhnyak¹; Andrew K. Ottens¹; ¹Dept Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA
- MP 701 **Asymmetric Flow Field-Flow Fractionation Coupled with On-Line Trypsin Digestion and LC-MS/MS for Quantitative Analysis of Lipoprotein Sub-Class Composition;** John R. Barr¹; Zsuzsanna Kuklenyik²; Michael Gardner²; Bryan A Parks²; Christopher Toth³; Jeffrey Jones²; Michael Andrews³; David M Schieltz²; Jon Rees²; Lisa G McWilliams²; James L. Pirkle²; ¹CDC, Atlanta, GA; ²Center for Disease Control and Prevention, Atlanta, GA; ³Battelle Memorial Institute, Atlanta, GA
- MP 702 **Analysis of Liver and Heart Spheroids in Drug-Induced Hepatotoxicity and Cardiotoxicity;** Nathalie Selevsek¹; Bernd Roschitzki¹; Jens Kelm²; Olivia Rose Clayton³; Claudia Fortes¹; Witold Wolski¹; Jonas Grossmann¹; Laura Kunz¹; Paolo Nanni¹; Adrian B. Roth³; Ralph Schlapbach¹; ¹Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; ²InSphero AG, Schlieren, Switzerland; ³Roche Innovation Center Basel, Grenzacherstrasse Basel, Switzerland
- MP 703 **Label Free Proteomics Profiling Unveils Down Regulation of Thrombin Mediated Signaling and Aggregation of Human Platelets upon Treatment with Thrombin Inhibitors;** Cristina Clement¹; Ebenezer L.V. Ewul²; Anna Babinska³; Janet Gonzalez⁴; Monika Dzieciatkowska^{5,6}; Moro Salifu⁷; Manfred Philipp²; ¹Albert Einstein CollegeMed, Bronx, NY; ²Chemistry Department Lehman College CUNY, Bronx, NY; ³Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY; ⁴Department of Natural Sciences, LaGuardia Community College, Queens, NY; ⁵Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Colorado; ⁶Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Denver, CO; ⁷Division of Nephrology, Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY
- MP 704 **Validation of a Unified Sample Preparation Platform for Multi-Omics Technologies;** Danielle Gutierrez¹; Stacy D Sherrod¹; Jeremy L Norris¹; Carrie E Romer¹; Melissa A Farrow¹; Simona Codreanu¹; Randi Lee Gant-Branum¹; Yuan-wei Nei¹; John A McLean¹; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN
- MP 705 **ChIP-MS/TMT: A Quantitative Proteomic Analysis of Steroid Hormone Receptor Activation;** Andrew Holding¹; , Cambridge, Cambridgeshire
- MP 706 **Proteomewide Profiling of Geranylgeranyl Pyrophosphate-Protein Interaction Network in Liver via Click Chemistry-Based Affinity Purification and Mass Spectrometry;** Lei Fang¹; Jingzi Zhang¹; Di Shen¹; Bin Xue¹; Lan Huang²; Chaojun Li¹; ¹Nanjing University, Nanjing, China; ²University of California-Irvine, Irvine, CA
- MP 707 **Novel Method to Process Proteomics for Identification of Pathways Associated with Anti-Colon Cancer Properties of Anthocyanin-Rich Purple-Fleshed Potato in Mice;** Venkata Charepalli¹; Vadiraja Bhat²; Lavanya Reddivari³; Jairam Vanamala^{3,4}; ¹Pennsylvania State University, University Park, Pennsylvania; ²Agilent Technologies, Wilmington, DE; ³The Pennsylvania State University, State College, PA; ⁴The Penn State Hershey Cancer Institute, Hershey, PA

TOP DOWN PROTEIN ANALYSIS (APPLICATIONS) 708 – 727

- MP 708 **TopDownLab – Proteoform-Specific Monitoring of Multi-Site Protein Phosphorylation;** Andrea Mizzi Brunner¹; Philip Lössl¹; Albert J R Heck¹; Maarten A F Altelaa¹; Richard A Scheltema¹; ¹Utrecht University, Utrecht, Netherlands
- MP 709 **Top-Down Proteomic Study of Sarcomere Protein Post-Translational Modifications in Aging Skeletal Muscle;** Liming Wei¹; Ziqing Lin¹; Yutong Jin²; Wenxuan Cai¹; Zachery R. Gregorich¹; Ying Ge¹; ¹Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison; ²Department of Chemistry, University of Wisconsin-Madison, Madison

- MP 710 **Ultra-Fast Analysis of Hemoglobin Isoforms Using Capillary Electrophoresis Coupled to Mass Spectrometry and Ultraviolet Photodissociation;** Andreas Krupke¹; Chien-Hsun Chen¹; Xiaolei Xie¹; Chad R Weisbrod¹; Romain Huguet¹; Shiaw-Min Chen²; Achim Karger²; Steve Williams²; Michael Wenz²; Andreas Huhmer¹; Aran Paulus¹; Daniel Lopez-Ferrer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, South San Francisco, CA
- MP 711 **Evaluation and Application of Top-Down Mass Spectrometry for Exploring the Low Molecular Weight Proteome of Osteosarcoma Cells;** Liping Yang¹; Zifeng Song¹; Claudia S Maier¹; ¹Oregon State University, Corvallis, OR
- MP 712 **Top-Down Mass Spectrometry Applications for Detection of N-Terminal Sequence Heterogeneity and PTMs for a Therapeutic Molecule;** Bao Quoc Tran¹; Shivangi Awasthi¹; Mohd M Khan¹; David R Goodlett¹; Young Ah Goo¹; ¹University of Maryland Baltimore
- MP 713 **Targeted Intact Protein Fragmentation in Complex Mixtures Using a Charge State Scheduled Precursor List of Regulated Proteoforms;** Jim Kapron¹; Rainer Paape²; Markus Lubeck²; Schmit Pierre-Olivier³; ¹Bruker Ltd, Vancouver, Canada; ²Bruker Daltonic GmbH, Bremen, Germany; ³Bruker Daltonique S.A., Wissembourg, bas-rhin
- MP 714 **Investigating Binding Sites of Metal Drugs to Ubiquitin Using Free-Access chemInfo.org Algorithms;** Laure Menin¹; Ronald F.S. Lee²; Luc Patiny²; Daniel Ortiz²; Paul J. Dyson²; ¹EPFL SB ISIC-GE, Lausanne; ²EPFL, Lausanne, Switzerland
- MP 715 **Human Proteoform Identification by Top-Down LC-MS/MS Utilizing a 21 Tesla FT-ICR Mass Spectrometer;** Lissa C Anderson¹; Caroline J DeHart¹; Nathan K Kaiser¹; Donald F Smith¹; Christopher L Hendrickson¹; ¹NHMF, Tallahassee, FL
- MP 716 **Top-down MS/MS Analysis of Canonical Histone H2A Phosphorylation During the Cell Cycle;** Xibei Dang¹; Michael E Hoover²; Chen Yu³; Alan G Marshall^{4,5}; Michael A Freitas²; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Ohio State University, Columbus, OH; ³University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ⁴National High Magnetic Field Laboratory, Tallahassee, FL; ⁵Florida State University, Tallahassee, Florida
- MP 717 **Comprehensive, Quantitative Intact Proteoform Measurements of Patient-Derived Breast Tumor Xenografts Using an Improved Top-Down Proteomics Pipeline;** Tao Liu¹; Paul D Piehowski¹; Samuel H Payne¹; Sangtae Kim¹; Jungkap Park¹; Christopher S Wilkins¹; Carrie D Nicora¹; Yufeng Shen¹; Rui Zhao¹; Anil K Shukla¹; Ronald J Moore¹; Sherri R Davies²; Shunqiang Li²; Reid R Townsend²; Matthew J Ellis³; Emily S Boja⁴; Henry Rodriguez⁴; Karin D Rodland¹; Richard D Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Washington University, St Louis, MO; ³Baylor College of Medicine, Houston, TX; ⁴National Cancer Institute, Bethesda, MD
- MP 718 **Top-Down LC/MS Analysis of Myofilament Proteoforms in Dilated Cardiomyopathy;** Yumin Lian¹; Ziqing Lin¹; Yi-Chen Chen¹; Nicole Marie Lane¹; Takushi Kohmoto¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 719 **YahO Protein as a Calibrant For Top-Down Proteomic Identification of Shiga Toxin Using MALDI-TOF-TOF-MS/MS and Post-Source Decay;** Clifton K. Fagerquist¹; William James Zaragoza¹; ¹USDA/ARS, Albany, CA
- MP 720 **Label-Free Quantitative Analysis of Mouse Brain Proteoforms Using Top Down Proteomics;** Roderick G. Davis¹; Kyunggon Kim¹; Paul M Thomas¹; Ryan T Fellers¹; Richard D Leduc¹; VanNispen J Alexandra¹; Jonathan Sweedler²; Justin Rhodes²; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- MP 721 **Assessing Organismal and Spatial MBP Proteoform Diversification in Healthy Rats by Top-Down Mass Spectrometry (TDMS);** Casey E Wing¹; Micheal Tran¹; Daniel A Plymire²; John Corbett^{1,2}; Steven M Patrie^{1,2}; ¹University of Texas at Dallas, Richardson, TX; ²University of Texas Southwestern Medical Center, Dallas, TX
- MP 722 **Top-Down Proteomics can Differentiate Closely Related Pathogenic Enterobacteria;** Mathieu Dupré¹; Valeria Calvaresi¹; Christian Malosse¹; Magalie Duchateau¹; Dominique Clermont¹; Julia Chamot-Rooke¹; ¹Institut Pasteur, Paris, France
- MP 723 **Analysis of Proteoforms in Membrane Protein Complexes by Top-Down Proteomics;** Hans JCT Wessels¹; Sergio Guerrero-Castillo¹; Roel Tans¹; Schmit Pierre-Olivier²; Stuart Pengelley³; Alain J Van Gool¹; ¹Radboudumc, Nijmegen, Netherlands; ²Bruker Daltonique S.A., Wissembourg, bas-rhin; ³Bruker Daltonic GmbH, Bremen, Germany
- MP 724 **Top Down 3D Spatial Mapping of Myelin Basic Protein Proteoforms: Organism and Spatial Diversification and its Potential Impact on Auto Immunity;** Daniel Plymire¹; John Corbett^{1,2}; Casey Wing^{1,2}; Michael Tran^{1,2}; Steven Patrie^{1,2}; ¹University of Texas Southwestern Medical Center, Dallas, TX; ²University of Texas at Dallas, Richardson, TX
- MP 725 **Preparing to Read the Ubiquitin Code: Top-Down Analysis of Polyubiquitin Chains;** Amanda Lee¹; Lucia Geis-Asteggianti¹; Emma Dixon¹; Tanuja Kashyap¹; Yan Wang¹; David Fushman¹; Catherine Fenselau¹; ¹University of Maryland, College Park, MD
- MP 726 **Identification of Secretory Virulence Factors in S. aureus by Combination of Proteomics Methods;** Santosh Misal¹; Shital D Ovhal¹; Jonathan A Karty¹; James P Reilly¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- MP 727 **Top-Down High Resolution Accurate Mass-Mass Spectrometry for Identification of Clinical Yeast Species;** Joanna Freeke¹; Azadeh Jamalian²; Mansoureh Vatanashenassan²; Bert Gerrits van den Ende²; Helene L Cardasis³; Johan Finell⁴; Ping F. Yip³; Scott R. Kronewitter³; James Jr L Stephenson³; Alexander Y. Cherkassky³; J. Benjamin Stielow¹; Sybren de Hoog²; ¹Thermo Fisher Scientific, Utrecht, Netherlands; ²CBS-KNAW Fungal Biodiversity Center, Utrecht, Netherlands; ³Thermo Fisher Scientific, Cambridge, MA; ⁴Thermo Fisher Scientific, Vantaa, Finland

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

Antibodies & Antibody Drug Conjugates (Separations)	001 - 028
Biomarkers: Quantitative Analysis (Part 1)	029 - 054
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling (Cross-Linking)	055 - 075
Data Independent Acquisition (SWATH)	076 - 095
Diagnostic Clinical Chemistry (General)	096 - 112
Drug Discovery/DMPK/ADME (Applications)	113 - 129
Drug Metabolism: Qualitative and High Throughput Analysis	130 - 144
Energy: Hydrocarbon and Petrochemical (Hi Res and Nominal)	145 - 163
Environmental Analysis: General (Part 2)	164 - 188
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Food Safety (Pesticides in Food)	210 - 235
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Forensics (Part 1)	251 - 278
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High Mass Accuracy/High Performance MS Methods & Developments	297 - 312
Imaging MS: Disease Markers	313 - 344
Imaging MS: Pharmaceutical Applications	345 - 363
Informatics: Peptide ID and Quantification	364 - 391
Instrumentation: General	392 - 416
Instrumentation: New Developments in Mass Analyzers	417 - 442
Ion Mobility: Applications (Proteins & Peptides)	443 - 470
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Metabolomics: Untargeted Metabolite Profiling (Cells/Plants)	530 - 557
Nucleic Acids	558 - 582
Peptides: PTM Identification	583 - 605
Phosphopeptides: Quantitative Analysis	606 - 623
Proteins: Complexes/Non-covalent Interactions	624 - 659
Proteomics: Clinical Applications (Development toward Clinical Application)	660 - 681
Proteomics: Infectious Diseases	682 - 702
Proteomics: Quantitative (Application Biological Research)	703 - 727
Small Molecules: Quantitative Analysis (Animal, Plant/Insect, and Methodology)	728 - 762
Top Down Protein Analysis (Methodology)	763 - 775

ANTIBODIES & ANTIBODY DRUG CONJUGATES (SEPARATIONS) 001 - 028

- TP 001 **A Sensitive Multidimensional Liquid Chromatography Method for the Characterization of Free Drug Impurities in Antibody-drug Conjugates using Mass Spectral Detection;** Robert Birdsall¹; Sean M McCarthy²; Alain Beck³; John Gebler²; Weinbin Chen²; ¹Waters Corporation, Milford, MA; ²Waters, Milford, MA; ³Pierre Fabre, St Julien-en-Genevois, France
- TP 002 **Characterization and Spectral Library Building of Glycopeptides in the Tryptic Digest of a Monoclonal Antibody Using 1D and 2D LC-MS/MS;** Qian Dong¹; Xinjian Yan²; Yuxue Liang²; Stephen Stein²; ¹NIST, Gaithersburg, MD; ²NIST, Rockville, MD
- TP 003 **DAR Calculation of Cysteine Linked ADCs by Reversed Phase High Performance Liquid Chromatography Tandem High Resolution mass spectrometry;** Shuai Zuo¹; Tao Bo¹; ¹Agilent Technologies (China) Limited, Beijing, China

- TP 004 **Characterization of Antibody Drug Conjugate: Intact, Fragment and Peptide Mapping using Reversed Phase Columns;** Suresh Babu Cv¹; Tang Ning²; Anne Blackwell³; ¹Agilent Technologies, Bangalore, Karnataka; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Little Falls, DE
- TP 005 **Comparison of Innovator and Biosimilar by Peptide Mapping using HPLC Coupled to Time-of-Flight Mass spectrometry;** Ravindra Gudihal¹; Ning Tang²; ¹Agilent Technologies India Pvt. Ltd, Bangalore, Karnataka; ²Agilent Technologies, Santa Clara, CA
- TP 006 **Towards the Complete Characterization of Host Cell Proteins in Biotherapeutics via Affinity Depletions, LC-MS/MS, and Multivariate Analysis;** Jennifer Murphy¹; James A. Madsen¹; Victor Farutin²; Yan Yin²; Stephen Smith²; James Anderson²; Ishan Capila²; ¹Momenta Pharmaceuticals, Cambridge, MA; ²Momenta Pharmaceuticals, Cambridge, ma
- TP 007 **Reversed-Phase Separation of Therapeutic Monoclonal Antibodies Using Superficially Porous Column: LC/MS Analysis;** Suresh Babu Cv¹; Ning Tang²; Anne Blackwell³; ¹Agilent Technologies, Bangalore, Karnataka; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Little Falls, DE
- TP 008 **Rapid Automated LC-MS/MS Glycan Analysis for Monoclonal Antibodies;** Bhavana Shah¹; Jason Richardson²; Zhongqi Zhang²; ¹Amgen Inc., Thousand Oaks, CA; ²Amgen, Inc., Thousand Oaks, CA
- TP 009 **Towards the Automated Monoclonal Antibody Sequencing and Characterization from LC-MS data;** Lin He¹; Mohammad Ziaur Rahman¹; Ngoc Hieu Tran²; Baozhen Shan¹; Ming Li²; ¹Bioinformatics Solutions Inc., Waterloo, Canada; ²David R. Cheriton School of Computer Science, University of Waterloo, Waterloo, ON
- TP 010 **Development of a Non-Toxic Antibody Drug Conjugate Mimic to Enable LC-MS Method Development Without Risk;** Kevin Ray¹; Brian Gau¹; John Dapron¹; Nicolas Caffarelli¹; Jeffrey Turner¹; ¹MilliporeSigma, St Louis, MO
- TP 011 **Characterisation of Antibody Conjugates under Denaturing Liquid Chromatography Mass Spectrometry (MS) and Native MS Conditions;** Kersti Karu^{1,2}; Maurício Moraes²; James R Baker²; ¹UCL Chemistry Mass Spectrometry Facility, London; ²Department of Chemistry, Christopher Ignold Building, London, UK
- TP 012 **Electrospray-Ionization Time-of-Flight Mass Spectrometry Coupled to Online, Comprehensive Two-Dimensional Liquid Chromatography for the Characterization of Therapeutic Monoclonal Antibodies;** Matthew Sorensen¹; David Christopher Harnes¹; Gregory O Staples²; Szabolcs Fekete^{3,4}; Davy Guillaume^{3,4}; Alain Beck⁵; Dwight Stoll¹; ¹Gustavus Adolphus College, Saint Peter, MN; ²Agilent Technologies, Santa Clara, CA; ³University of Geneva, Geneva, Switzerland; ⁴University of Lausanne, Geneva, Switzerland; ⁵Center for Immunology Pierre Fabre, Saint-Julien-en-Genevois, France
- TP 013 **Native Liquid Chromatography-Mass Spectrometry Applied to the Validation of Drug to Antibody Ratio LC-UV Methods and Antibody Drug Conjugates Development;** Lieza Danan-Leon¹; Guillaume Tremintin²; ¹stemcentrx, South San Francisco, CA; ²Bruker Daltonics, Fremont, CA
- TP 014 **Direct Analysis of Intact mAb's and Low Abundant Variants by Advanced LC-MS Approaches;** Xiaomei (Annie) He¹; Janet Lau; Chen Li; Shiao-Lin Wu; ¹BioAnalytix, Cambridge, MA
- TP 015 **Mass Spectrometric Characterization of Half-mAb Separated from Intact Monoclonal Antibody and Fragments using Analytical Size Exclusion Chromatography Column;** Crystal Benner¹; William Evans¹; Cesar Zuin¹; Kyle Root²; Kerney Jebrell Glover³;

- TP 016 **LC-MS Characterization of Proteolytic Cleavage Sites in Therapeutic Monoclonal Antibodies**; Pavel V. Bondarenko¹; Thomas M Dillon¹; Gang Xiao²; Nicole Ball¹; Deirdre M Piedmonte¹; Michael J Treuheit¹; ¹Amgen, Inc., Thousand Oaks, CA; ²Amgen, Inc., Thousand Oaks, CA
- TP 017 **Probing Higher-Order Structural Changes of a Lysine-linked Antibody-Drug Conjugate by Hydrogen-deuterium Exchange Mass Spectrometry (HDXMS)**; Lintao Wang¹; Alexandru C. Lazar²; ¹ImmunoGen Inc., Waltham, MA; ²ImmunoGen, Inc., Waltham, MA
- TP 018 **A New Workflow for Characterization of Antibody Mixtures via Slip Flow Chromatography and Ultraviolet Photodissociation for Top-Down Mass Spectrometry**; Luca Fornelli¹; Philip Compton¹; Ximo Zhang²; Mary Wirth²; Neil Kelleher¹; ¹Northwestern University, Evanston, IL; ²Purdue University, West Lafayette, IN
- TP 019 **Glycoform Separation and Characterization of Cetuximab Variants by Middle-up Off-line CE-UV/ESI-MS**; Nassur Said¹; Michael Biacchi¹; Rabah Gahoual^{1,2}; Charly Renard¹; Alain Beck³; Yannis-Nicolas Francois¹; Emmanuelle Leize-wagner¹; ¹Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; ²Division of BioAnalytical Chemistry, AIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherlands; ³Centre d'Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France
- TP 020 **High-order Structural Interrogation of Antibody-drug Conjugates by a Combination of Intact, Middle-up and Bottom-up Techniques using Sheathless Capillary Electrophoresis-Mass Spectrometry**; Nassur Said¹; Rabah Gahoual^{1,2}; Laurianne Kuhn³; Alain Beck⁴; Yannis-Nicolas Francois¹; Emmanuelle Leize-wagner¹; ¹Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; ²Division of BioAnalytical Chemistry, AIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherlands; ³Institut de Biologie Moléculaire et Cellulaire (IBMC), University of Strasbourg, Strasbourg, France; ⁴Centre d'Immunologie Pierre-Fabre, St. Julien-en-Genevois, France
- TP 021 **Microchip Capillary Electrophoresis with Integrated ESI-MS for the Detailed Analysis of Intact Biotherapeutic Antibodies and ADCs**; J. Scott Mellors¹; Erin Anne Redman²; J. Michael Ramsey²; ¹908 Devices, Inc., Chapel Hill, NC; ²University of North Carolina, Chapel Hill, NC
- TP 022 **Capillary Electrophoresis – Mass Spectrometry for Top Down Proteomics**; Andreas Krupke¹; Shiaw-Min Chen²; Achim Karger²; Michael Wenz²; Daniel Lopez-Ferrer²; Aran Paulus²; ¹Thermo Fisher Scientific, South San Francisco, CA; ²Thermo Fisher Scientific, San Jose, CA
- TP 023 **Intact Immunoglobulin Gamma Analysis by CESI-MS**; Bryan Fonslow^{1,2}; Olga Friese³; Ying Zhang³; John Yates III²; K. Steven Cook³; Jason Rouse⁴; ¹SCIEX, San Diego, CA; ²The Scripps Research Institute, La Jolla, CA; ³Pfizer, Chesterfield, MO; ⁴Pfizer, Inc. Andover, MA
- TP 024 **Characterization of Monoclonal Antibody Charge Variants using OFFgel Fractionation and Mass Spectrometry**; Alyssa Neill¹; Yekaterina Kori²; Guilong Charles Cheng¹; Hongcheng Liu¹; ¹Alexion Pharmaceuticals Inc., New Haven, CT; ²University of Massachusetts Amherst, Amherst, Massachusetts
- TP 025 **Bioanalytical Challenges of Next-Generation Antibody-Drug-Conjugates Case Study: Developing a 2nd-Generation Affinity Capture LC-MS to Improve In Vivo Stability Assessment**; Dian Su; Genentech Inc, South San Francisco, CA
- TP 026 **Novel Microfluidic Chip with In-line Deglycosylation for Rapid Mass Analysis of Reduced Monoclonal Antibodies**; Loredana Serafini¹; John Corbin¹; Victoria Smith¹; Mark Nagel¹; Leanna Laggapan¹; Debi Jin¹; Andy Gieschen²; Caroline S. Chu²; Katherine Brenda¹; ¹Gilead Sciences, Foster City, CA; ²Agilent Technologies, Santa Clara, CA
- TP 027 **Multidimensional ionKey/MS for Antibody Drug Conjugate Analysis**; Greg Roman¹; James P Murphy¹; ¹Waters, Milford, MA
- TP 028 **Using Hydrophilic Interaction Chromatography–Mass Spectrometry for Heightened Product Characterization to Overcome Challenges with Hydrophobic Antibodies and Antibody Drug Conjugates**; Jacquelyn Smith¹; Matthew Lauber²; Stephan Koza²; Erin Chambers²; Jason C Rouse³; Olga Friese⁴; ¹Senior Associate Scientist at Pfizer, Chesterfield, MO; ²Waters, Milford, MA; ³Pfizer, Inc. Andover, MA; ⁴Pfizer, Chesterfield, MO
- BIOMARKERS: QUANTITATIVE ANALYSIS (PART 1)**
029 - 054
- TP 029 **Towards Absolute Quantification of Protein Expression in 3D Tissue Culture Samples by MALDI-IMS-MS Imaging**; Rebecca Day¹; Amanda Harvey¹; Laura M Cole¹; Neil Cross¹; David Smith¹; Malcolm Clench¹; ¹Sheffield Hallam University, Sheffield, United Kingdom
- TP 030 **Double Standards in Proteomics: DOSCATS: Engineered Peptide/Epitope Concatenations for SRM or Western Blotting**; Robert Beynon¹; Richard J Bennett¹; Deborah M Simpson¹; Stephen W Holman¹; John Colyer^{2,3}; ¹University of Liverpool, Liverpool, United Kingdom; ²University of Leeds, Leeds, United Kingdom; ³Badrilla Ltd., Leeds, UK
- TP 031 **Development of New LC-MS Methodologies to Assess Liver Function in a Clinical Setting using Plasma and Dried Blood Spot**; Lei Guo¹; Raymond Gonzalez¹; Kara Pearson¹; Elizabeth Joshi²; Kevin P Bateman¹; Daniel S Spellman¹; ¹Merck & Co., Inc., West Point, PA; ²Merck & Co, Kenilworth, NJ
- TP 032 **Serial Lectin Affinity Chromatography for Comparative Serum Glycoproteomics on Colon Cancer Biomarker Discovery**; Jinwook Lee¹; Wonryeon Cho¹; ¹wonkwang University, Iksan, Jeonbuk
- TP 033 **Between Good, Fast and Cheap: Method Development for Large-Scale Plasma-Proteome Analysis between the Antagonizing Poles of Sensitivity, Through-put and Costs**; Christoph Stingl¹; Lennard Dekker¹; Diana A T Nijholt¹; Coskun Güzel¹; Martijn M. van Duijn¹; Theo M. Luider¹; ¹Erasmus Medical Center, Rotterdam, The Netherlands
- TP 034 **Comparative Proteomic Analysis of Kidney Distal Convoluted Tubule and Cortical Collecting Duct Cells following Long-Term Hormonal Stimulation**; Qi Wu¹; Trairak Pisitkun²; Robert Fenton¹; ¹Center for Interactions of Proteins in Epithelial Transport, Department of Biomedicine, Aarhus, Denmark; ²Faculty of Medicine, Chulalongkorn University, Bangkok, Thailand
- TP 035 **Higher Protein Identifications and Coverage May Not Correlate with Higher Numbers of PSMs or Peptides in Quantitative Proteomic Analyses**; Lauren Devine¹; Tatiana Boronina¹; Robert N O'Meally¹; Robert N Cole¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
- TP 036 **Identification of Pathological-Synuclein Forms in Brain Extracts from Patients with Parkinson's Disease by Selected Reaction Monitoring**; Pavel Bhattacharjee¹; Ann Brinkmalm¹; Annika Öhrfelt¹; Kaj Blennow¹; Henrik Zetterberg¹; ¹University of Gothenburg, Mölndal, Sweden
- TP 037 **Development of a TFPI (Tissue Factor Pathway Inhibitor) Protein Quantification Assay**; Katherine Wright; Pfizer, Andover, MA

- TP 038 **A High-throughput Platform for Mass Spectrometric Analysis of Serum Fucosylated Haptoglobin in Hepatocellular Carcinoma;** Jianhui Zhu¹; Jing Wu¹; Haidi Yin¹; Jorge Marrero²; David M Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Texas Southwestern Medical Center, Dallas, TX
- TP 039 **Development of Plasma Protein Biomarkers for Effects of Radiation Exposure Using Quantitative Mass Spectrometry;** Kate Liu¹; Dyna Shirasaki¹; Elizabeth Singer¹; William McBride¹; Julian Whitelegge¹; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA
- TP 040 **Phosphoproteomic Analysis of Differential Protein Expression in BRAF-Mutated Melanoma Cells with Acquired Resistance to BRAF, MEK1/2, or ERK1/2 Inhibitors;** Shivangi Awasthi¹; Jacob Sheenstra¹; Bao Tran¹; Young Ah Goo¹; Paul Shapiro¹; David R Goodlett¹; ¹University of Maryland Baltimore, Baltimore, USA
- TP 041 **Identification of Novel Glycoprotein Biomarkers for Distinguishing Intestinal Inflammation from Fibrosis in Crohn's Disease by LC-MS/MS;** David M Lubman¹; Jing Wu¹; Ryan Stidham¹; Peter Higgins¹; Henry Appelman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- TP 042 **LC-MS/MS Method for Quantitation of Seven Biomarkers in Human Plasma for the Assessment of Impaired Glucose Tolerance;** Qibo Zhang¹; Lisa A Ford¹; Kelli D Goodman¹; Tiffany A Freed¹; Deirdre M Hauser¹; Jessie K Conner¹; Kate E T Vroom¹; Klaus-Peter Adam¹; Michael V Milburn¹; Douglas R Toal¹; ¹Metabolon, Inc., Durham, NC
- TP 043 **A Robust Analytical LC-MS/MS Method to Quantitate Plasma Itraconazole and Hydroxy-itraconazole in Patients with Solid Tumors;** Claudia Meek¹; Erling Beck¹; Richard Leff²; ¹Texas Tech University, Dallas, TX; ²Texas Tech University Health Sciences Center, Dallas, TX
- TP 044 **Investigation of the Quantitative Properties of Micro Flow LC-MS/MS for Direct Analysis of Frataxin in Human Biopsy;** Qishan Lin¹; Jinghua Zhu²; ¹University at Albany, Rensselaer, NY; ²University at Albany, Rensselaer, NY
- TP 045 **Ultra high Performance Liquid Chromatography-Tandem Mass Spectrometry (UHPLC-MS/MS) Platform for Clinical Diagnostics within Diabetes Care;** Linda Ahonen¹; Sirkku Jäntti²; Matej Orešič¹; Tuulia Hyötyläinen¹; ¹Steno Diabetes Center A/S, Gentofte, Denmark; ²University of Helsinki, Helsinki, Finland
- TP 046 **Quantitative Discovery of the Alterations of the Entire Human Kinome in Human Cells upon Methylglyoxal Treatment;** Weili Miao¹; Lei Guo¹; Yongsheng Xiao¹; Xiaogang Jiang¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA
- TP 047 **A Comprehensive Investigation towards the Indicative Proteins of Bladder Cancer in Urine: From Surveying Cellular Secretomes to Verifying Urine Proteins;** Jiao Guo¹; ¹Beijing, Beijing
- TP 048 **Development of MS Based Clinical Assays for Measuring Cerebrospinal Fluid Levels of Pre-Synaptic Proteins in Alzheimer's Disease;** Ann Brinkmalm¹; Gunnar Brinkmalm¹; Henrik Zetterberg^{1,2}; Kaj Blennow¹; Annika Öhrfelt¹; ¹University of Gothenburg, Mölndal, Sweden; ²UCL Institute of Neurology, London, UK
- TP 049 **Quantification of Hepcidin-25 in human Cerebrospinal Fluid using LC-MRM;** Jerome Vialaret¹; Constance Delaby¹; Pauline Bros^{1,2}; Amandine Moulinier¹; Vincent Delatour³; Audrey Gabelle⁴; Sylvain Lehmann¹; Christophe HIRTZ¹; ¹LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; ²Laboratoire National de Métrologie et d'Essais, Paris, France; ³Laboratoire National de Métrologie et d'Essais, Paris, France; ⁴Centre Mémoire Ressources CHRU Montpellier, Montpellier, France
- TP 050 **Measurement of DNA Repair Protein Apurinic/ Apyrimidinic Endonuclease 1 (APE1) in Human Tissues by Liquid Chromatography/Tandem Mass Spectrometry with Isotope Dilution;** Pawel Jaruga¹; Fatos Guldal Kirkali²; Prasad T. Reddy³; Alessandro Tona³; Bryant C. Nelson³; Mengxia Li⁴; David M. Wilson, III⁵; Erdem Coskun⁶; Miral Dizdar⁶; ¹NIST, Gaithersburg, MD; ²NIH/NCI (National Cancer Institute), Bethesda, MD; ³NIST, Gaithersburg MD; ⁴NIH/NIH/IRP, Baltimore, MD; ⁵NIH/NIH (National Institute on Aging), Baltimore, MD; ⁶NIST, Rockville, MD
- TP 051 **Phosphoproteome Analysis Reveals Differential Mode of Action of Sorafenib in Wildtype and Mutated FLT3 AML Cells;** Catrin Roof¹; Nikolaj Dybowski²; Anett Sekora¹; Stefan Mueller²; Gudrun Knuebel¹; Hugo Murua Escobar¹; Klaus Godt²; Andreas Tebbe²; Christian Junghans¹; Christoph Schaab²; ¹Rostock, University Medical Center, Department of Hematology/ Oncology/ Palliative Care, Rostock, Germany; ²Evotec (München) GmbH, Munich, Germany
- TP 052 **Improved Quantification of Rat Plasma NNK and NNAL Using Protein Precipitation and Phospholipid Removal in UFLC-ESI/MS/MS;** Efstathia Sepehr¹; Matthew S Bryant²; ¹National Center for Toxicological Research, FDA, Jefferson, AR; ²National Center for Toxicological Research - FDA, Jefferson, AR
- TP 053 **Accurate Quantification of Peptide using Multiple Internal Standards in Conjunction with parallel reaction monitoring;** Sebastien Gallien¹; Bruno Doman¹; ¹Luxembourg Clinical Proteomics Center, Strassen, Luxembourg
- TP 054 **Precise MRM-based Quantitation of 200 Proteins from Dried Blood Spots and Single Drops of Blood;** Jingxi Pan¹; Suping Zhang²; Albert Chou¹; Christoph H. Borchers^{3,4}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²MRM Proteomics, Inc., Victoria, BC, Canada; ³University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING (CROSS- LINKING) 055 - 075

- TP 055 **The Synaptic Vesicle Cycle is Governed by Heterogeneous and Macromolecular Protein Microdomains;** Carla Schmidt¹; HALOmem, University of Halle, Halle / Saale
- TP 056 **Structure of α -Synuclein Determined by Structural Proteomics and Constraint-Driven Discrete Molecular Dynamic Modeling;** Nicholas I Brodie¹; Konstantin I Popov²; Evgeniy V Petrotchenko¹; Nikolay V Dokholyan²; Christoph H. Borchers^{1,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²University of North Carolina, School of Medicine, Chapel Hill, NC; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- TP 057 **Profiling Yeast Mitochondrial Protein-Protein Interactions in a Whole-Organellar Scale by Cross-Linking Mass Spectrometry;** Chung-Tien Lee^{1,2}; Peter Rehling²; Henning Urlaub^{1,2}; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²University Medical Center (UMG), Goettingen, Germany
- TP 058 **Transcription Factor-DNA Interaction Studied by Structural Mass Spectrometry;** Lukas Slavata^{1,2}; Michal Rosulek^{1,2}; Daniel Kavan^{1,2}; Alan Kadek^{1,2}; Hynek Mrazek^{1,2}; Petr Man^{1,2}; Petr Novak^{1,2}; ¹Institute of Microbiology CAS, Prague, Czech Republic; ²Faculty of Science, Charles University in Prague, Prague, Czech Republic

- TP 059 **Assessing the Performance of CID-cleavable cross-linkers and Subsequent Data Analysis Strategies;** Rebecca Beveridge¹; Karl Mechtler¹; ¹Research Institute of Molecular Pathology (IMP), Vienna, Austria
- TP 060 **Improving Cross-linked Peptide Identification in Large Protein Complexes on Quadrupole-Orbitrap and Quadrupole-Orbitrap-Ion Trap Platforms;** Chung-Tien Lee¹; Olexandr Dybkov¹; Christof Lenz^{1,2}; Thomas Monecke³; Ralf Ficner³; Yue Xuan⁴; Henning Urlaub^{1,2}; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²University Medical Center (UMG), Goettingen, Germany; ³Georg August University, Goettingen, Germany; ⁴Thermo Fisher Scientific, Bremen, DE
- TP 061 **Optimization of Crosslinked Peptide Analysis on an Orbitrap Fusion Lumos Mass Spectrometer;** Ryan Bomgarden¹; Erum Raja¹; Chris Etienne¹; Fan Liu²; Albert J R Heck²; Mathias Mueller³; Rosa I Viner⁴; ¹Thermo Fisher Scientific, Rockford, IL; ²Utrecht University, Utrecht, The Netherlands; ³Thermo Fisher Scientific, Bremen, DE; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 062 **Structural Proteomics Analysis of the Native Tau Protein;** Karl A T Makepeace¹; Evgeniy V Petrotchenko¹; Christoph H. Borchers^{2,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, CANADA; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, CANADA
- TP 063 **Evaluation of a Photo-Activatable Unnatural Amino Acid Engineered Into Proteins To Crosslink And Identify interaction partners;** Robert Hettich¹; Chen Qian²; Steven King²; Melinda Hauser²; Jeffrey Becker²; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN
- TP 064 **Analysis of UV-induced DNA-protein cross-links in a chromatin model by mass spectrometry;** Alexandra Stuetzer¹; Christin Kappert¹; Aleksandar Chernev¹; Wolfgang Fischle^{1,2}; Henning Urlaub¹; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²KAUST, Thuwal, Saudi Arabia
- TP 065 **RNPxl 2 - Protein-RNA Interaction Site Localization from UV Cross-linked Peptide-RNA Oligonucleotides in Proteome Discoverer 2.1;** Timo Sachsenberg¹; Johannes Veit¹; Aleksandar Chernev²; Kundan Sharma²; Romina Hofele²; Saadia Qamar²; Uzma Zaman²; Christin Kappert²; Katharina Kramer³; Julianus Pfeuffer⁴; Xiao Liang⁴; Knut Reinert^{4,5}; Christof Lenz²; Henning Urlaub²; Oliver Kohlbacher^{1,6}; ¹Eberhard Karls University, Tübingen, Germany; ²Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; ³Max Planck Institute for Plant Breeding Research, Köln, Germany; ⁴Freie Universität Berlin, Berlin, Germany; ⁵Max Planck Institute for Molecular Genetics, Berlin, Germany; ⁶Max Planck Institute for Developmental Biology, Tübingen, Germany
- TP 066 **Novel Workflow for Characterization of Non-Disulfide Protein Crosslinks in Normal and Cataractous Human Lens;** Ruiqiang Chen¹; Kristie L. Rose¹; Zhen Wang¹; Kevin Schey¹; ¹Department of Biochemistry and Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN
- TP 067 **New Methodology for the *in vivo* Identification of Protein Partners using Genetically Encoded Unnatural Amino Acids and Mass Spectrometry;** Mariana Fioramonte¹; Bing Yang²; Ana Gisele C Neves-Ferreira³; Lei Wang²; Fabio César Gozzo¹; ¹University of Campinas, Campinas, Brazil; ²UCSF, San Francisco, CA; ³Fiocruz, Rio de Janeiro, RJ
- TP 068 **Systematic Determination of Nuclear Pore Complex Protein Interfaces by XL-MS;** Joseph Glavy¹; Martin Beck²; ¹Stevens Institute of Tech., Hoboken, NJ; ²EMBL Heidelberg, Heidelberg, Germany
- TP 069 **Quantitative Cross-linking/LCMS (CX-MS) to Investigate Allosteric Regulation of Phosphodiesterase 6 (PDE6);** Donna Hogan¹; Xiongzhuo Gao¹; Suzanne Matte¹; Rick Cote¹; Feixia Chu¹; ¹University of New Hampshire, Durham, NH
- TP 070 **Developing a Novel Multiplexed Quantitative Cross-linking Mass Spectrometry Strategy to Define the Structural Dynamics of Cullin-RING Ligase Complex;** Clinton Yu¹; Haibin Mao²; Alex Huszaghi¹; Rosa I Viner³; Eric Novitsky¹; Tonya Second³; Scott Rychnovsky¹; Ning Zheng²; Lan Huang¹; ¹University of California, Irvine, Irvine, CA; ²University of Washington, Seattle, WA; ³Thermo Fisher Scientific, San Jose, CA
- TP 071 **Developing A Novel Acidic Residue Reactive and Sulfoxide-containing MS-cleavable Homobifunctional Cross-linker for Studying Protein-Protein Interactions;** Craig Bryant Gutierrez¹; Clinton Yu¹; Alex Huszaugh¹; Eric Novitsky¹; Scott Rychnovsky¹; Lan Huang¹; ¹UC-Irvine, Irvine, CA
- TP 072 **Structural Analysis of a Myotoxin-antimyotoxin Complex by Cross-linking, Mass Spectrometry and Bioinformatics;** Barbara S. Soares¹; Surza L. G. Rocha¹; Diogo B. Lima²; Bruno Lomonte³; Gilberto B Domont⁴; Jonas Perales¹; Richard H. Valente¹; Francisco Gomes-Neto¹; Ana Gisele Neves-Ferreira¹; ¹Oswaldo Cruz Institute, Fiocruz, Rio de Janeiro, Brazil; ²Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; ³Clodomiro Picado Institute, University of Costa Rica, San José, Costa Rica; ⁴Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil
- TP 073 **Photocrosslink Coupled with Mass Spectrometry on a Transmembrane Protein Pump using an Unnatural Amino Acid, Benzoylphenylalanine;** Thao Nguyen¹; Grzegorz Sabat²; Michael Sussman¹; ¹UW Madison, Madison, WI; ²UW-Madison, Madison, WI
- TP 074 ***In vivo* Conformational Dynamics of Hsp90 and Its Interactors;** Juan Chavez¹; Devin K Schweppe¹; Jimmy K Eng¹; James E Bruce¹; ¹University of Washington, Seattle, WA
- TP 075 **An Integrated Workflow for Analysis of Proteins and Protein Complexes based on Cross-Linking/Mass Spectrometry with an MS/MS Cleavable Cross-Linker;** Christian Arlt¹; Michael Goetze¹; Christian Ihling¹; Christoph Hage¹; Mathias Schaefer²; Andrea Sinz¹; ¹Martin-Luther-Universität, Halle-Wittenberg, Germany; ²Universität zu Köln, Greinstrasse, Germany

DATA INDEPENDENT ACQUISITION (SWATH) 076 - 095

- TP 076 **Large-scale Quantitative Measurements of Rat Brain Hippocampus Membrane Proteome in Prolonged Simulated Microgravity Model by 2D-SWATH® Mass Spectrometry;** Peibin Qin¹; Yun Wang²; Lihai Guo¹; Yongqian Zhang²; Wenhai Jin¹; Yulin Deng²; ¹Shanghai AB Sciex Analytical Instrument Trading Co., Ltd., China, Beijing, China; ²School of Life Science, Beijing Institute of Technology, China, Beijing, China
- TP 077 **An Novel Alignment Strategy for SWATH-MS to Generate Comprehensive Proteomics Data Matrices;** Hannes Luc Röst^{1,2}; Yansheng Liu¹; Giuseppe D'Agostino³; Matteo Zanella³; Pedro Navarro⁴; George Rosenberger¹; Ben Collins¹; Ludovic Gillet¹; Giuseppe Testa³; Lars Malmström¹; Ruedi Aebersold¹; ¹ETH Zurich, Zürich, Switzerland; ²Stanford University School of Medicine, Palo Alto CA; ³Department of Experimental Oncology, European Institute of Oncology (Istituto di Ricovero e Cura a Carattere Scientifico, IRCCS), Milan, Italy; ⁴Institute for Immunology, University Medical Center of the Johannes Gutenberg University Mainz, Mainz, Germany

- TP 078 **Assessing Proteome Organization by Native SEC Coupled to SWATH-MS;** Moritz Heusel¹; George Rosenberger¹; Robin Hafen¹; Ben C. Collins¹; Matthias Gstaiger¹; Ruedi Aebersold^{1,2}; ¹*Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland*; ²*Faculty of Science, University of Zurich Zurich, Switzerland*
- TP 079 **Understanding the Square-Wave Nature of Q1 Isolation for Data Independent SWATH® Acquisition;** Randy J. Arnold¹; Leroi Desouza¹; Christie Hunter²; Patrick Pribil¹; ¹*SCIEX, Concord ON, Canada*; ²*SCIEX, Redwood City, CA*
- TP 080 **Extending the Depth of Coverage in SWATH® Acquisition with Deeper Ion Libraries;** Joerg Dojahn¹; Nick Morrice²; Christie Hunter³; ¹*SCIEX, Darmstadt, Germany*; ²*SCIEX, Warrington, UK*; ³*SCIEX, Redwood City, CA*
- TP 081 **The Use of Smaller Q1 Isolation Windows Improves Reproducibility in SWATH Based Protein Quantification Even at Higher Spectral Acquisition Rate;** Dipankar Malakar¹; Faraz Rashid¹; Manoj Pillai¹; ¹*SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India*
- TP 082 **Identification and Quantitation of Glycopeptides by SWATH Acquisition;** Chi-Hung Lin¹; Christoph Krisp^{1,2}; Mark Molloy^{1,3}; ¹*Macquarie University, Sydney, Australia*; ²*Australian Proteome Analysis Facility, Sydney, Australia*; ³*Australian Proteome Analysis Facility, Sydney, Australia*
- TP 083 **Using Scanning SWATH Windows to Improve both Quantitative and Qualitative Data over Conventional SWATH and IDA Methodologies;** Nic Bloomfield¹; Michael Murphy¹; Gordana Ivosev¹; Stephen Tate¹; ¹*SCIEX, Concord ON, Canada*
- TP 084 **Glycopeptide SWATH Analysis – a Workflow for Quantification of Glycopeptides in Complex Samples;** Miloslav Sanda¹; Nathan Edwards²; Radoslav Goldman¹; ¹*Georgetown University, Lombardi Cancer Center Washington, DC*; ²*Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC*
- TP 085 **Scrutinization of Library Building for SWATH Analysis;** Katleen Van Steendam¹; Elisabeth Govaert¹; Maarten Dhaenens¹; Liesbeth Vossaert¹; Dieter Deforce¹; ¹*Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, BELGIUM*
- TP 086 **SWATH-MS Proteomics and Chemometrics to Study the Cardiovascular Disease;** Marcello Manfredi¹; Eleonora Conte²; Carmela Chiariello³; Elisa Robotti⁴; Elia Ranzato⁴; Simona Martinotti⁴; Eleonora Mazzucco⁴; Fabio Gosetti⁴; Annalisa Castagna³; Daniela Cecconi⁵; Oliviero Olivieri³; Emilio Marengo⁴; ¹*ISALIT-DISIT, University of Piemonte Orientale, Alessandria, Italy*; ²*ISALIT, spin-off DISIT, University of Piemonte Orientale, NOVARA, IT*; ³*Department of Medicine, University of Verona, Verona, Italy*; ⁴*DISIT, University of Piemonte Orientale, Alessandria, Italy*; ⁵*Department of Biotechnology, University of Verona, Verona, Italy*
- TP 087 **Make Love, Not War: Towards a Comprehensive Workflow for the Integrated Analysis of Transcriptomics and Proteomics Data;** Katleen Van Steendam¹; Elisabeth Govaert¹; Liesbeth Vossaert¹; Maarten Dhaenens¹; Filip Van Nieuwerburgh¹; Laura De Clerck¹; Dieter De Coninck¹; Dieter Deforce¹; ¹*Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium*
- TP 088 **Single Shot Deep DIA Methods with Optimal Coverage, Reproducibility and Quantification Precision;** Roland Bruderer¹; David Gomez-Valera²; Oliver M Bernhardt¹; Tejas P Gandhi¹; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland*; ²*Max Planck Institute for Biophysical Chemistry, Goettingen, Germany*
- TP 089 **Accelerating Data Independent Acquisition with Microflow Chromatography;** Christie Hunter¹; Nick Morrice²; ¹*SCIEX, Redwood City, CA*; ²*SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK*
- TP 090 **Proteome-wide Turnover Analysis Quantifies Genetic Impact in Down Syndrome;** Yansheng Liu¹; Christelle Borel²; Li Li³; Torsten Mueller¹; Paul Boersema⁴; Pierre-Luc Germain⁵; Giuseppe Testa⁵; Andreas Beyer³; Stylianos Antonarakis²; Ruedi Aebersold¹; ¹*Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland*; ²*Department of Genetic Medicine and Development, University of Geneva Medical School, and University Hospitals of Geneva, Geneva, Switzerland*; ³*University of Cologne, Cologne, Germany*; ⁴*Institute of Biochemistry, Department of Biology, ETH Zurich, Zurich, Switzerland*; ⁵*Department of Experimental Oncology, European Institute of Oncology, Milan, Italy*
- TP 091 **Rapid Ion Mobility Deconvolution for High-throughput Analysis of Structural Isomers;** Michael E Pettit¹; Matthew R Brantley¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*
- TP 092 **Phospholipid Analysis Utilising a Novel, Data Independent, Mode of Acquisition on a QTOF Instrument with a Scanning Quadrupole Mass Filter;** Jayne Kirk¹; Steven Lai²; Jason Wildgoose¹; Keith Richardson¹; Martin Green¹; Paul Doorbar¹; Witold Niklewski¹; Kirsten Craven¹; Mark Wrona³; ¹*Waters Corporation, Wilmslow, UK*; ²*Waters Corporation, Beverly, MA*; ³*Waters Corporation, Milford, MA*
- TP 093 **Data-independent Acquisition (DIA) Reveals Changes in Mouse Cardiac Proteome from SS-31 Drug Intervention;** Ying Sonia Ting¹; Ying Ann Chiao¹; Gennifer E Merrihew¹; Peter Rabinovitch¹; Michael J MacCoss¹; ¹*University of Washington, Seattle, WA*
- TP 094 **MS1 Based Quantification Optimization on DIA Methods on a Quadrupole-Orbitrap Mass Spectrometer;** Roland Bruderer¹; Yue Xuan²; Oliver M Bernhardt¹; Tejas Gandhi¹; Thomas Moehring²; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland*; ²*Thermo Fisher Scientific, Bremen, DE*
- TP 095 **Data-independent Acquisition Mass Spectrometry-Based Proteomics of Thyroid Cancer Allows Comprehensive Identification of Malignancy-Associated Changes;** Juan Martinez-Aguilar^{1,2}; Roderick Clifton-Bligh³; Mark Molloy^{2,4}; ¹*National Autonomous University of Mexico, Mexico city, MEXICO*; ²*Macquarie University, Sydney, Australia*; ³*Kolling Institute of Medical Research, Sydney, Australia*; ⁴*Australian Proteome Analysis Facility, Sydney, Australia*

DIAGNOSTIC CLINICAL CHEMISTRY (GENERAL) 096 - 112

- TP 096 **Touch Paper Spray Ambient Mass Spectrometry for Paper-based Immunoassays: Towards On-demand Diagnosis;** Suming Chen¹; Qiongqiong Wan¹; Abraham Kwame Badu-Tawiah¹; ¹*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH*
- TP 097 **Real Time and Accelerated Stability Studies of Testosterone Calibrators;** Linda Nagore¹; Ravi Orugunty¹; Isil Dilek¹; Uma Sreenivasan¹; ¹*Cerilliant Corporation, Round Rock, TX*
- TP 098 **Automated Sample Preparation of Whole Blood for Therapeutic Drug Monitoring and Diagnostics by LC-MS using a Commercial Autosampler;** Guenther Boehm¹; Christian Berchtold²; Götz Schlotterbeck²; Reto Bolliger³; ¹*CTC Analytics AG, Zwingen, BL*; ²*Fachhochschule Nordwestschweiz Hochschule für Life Sciences, Muttenz, Switzerland*; ³*CTC Analytics AG, Zwingen, Switzerland*
- TP 099 **Pharmacotherapy Monitoring and Clinical Diagnosis of Patients with APRT Deficiency Utilizing UPLC-MS/MS Assay;** Unnur Arna Thorsteinsdottir^{1,2}; Finnur Freyr Eiriksson^{1,2}; Hrafnhildur Runolfsdottir¹; Vidar Edvardsson³; Runolfur Pálsson^{1,3}; Margret Thorsteinsdottir^{1,2}; ¹*University of Iceland, Reykjavik, Iceland*; ²*ArcticMass, Reykjavik, Iceland*; ³*The National University Hospital of Iceland, Reykjavik, Iceland*

- TP 100 **Quantitative Analysis of Steroids in Serum using Ultra High Performance Liquid Chromatography-Tandem Mass Spectrometry**; Heng-Tao Dong¹; Man-Yu Zhang¹; Shan-An Chan²; ¹Agilent Technology, Inc. Shanghai, China; ²Agilent Technology, Inc. Taipei Taiwan, Taiwan
- TP 101 **Breath and Exhaled Breath Condensate Analyzes for Disease Diagnosis and Monitoring of Newborns by Mass Spectrometry**; Vladimir Frankevich¹; Vitaliy Chagovets¹; Natalia Starodubtseva¹; Alexey Kononikhin¹; Anna Bugrova¹; Andrey Ryndin¹; Oleg Ionov¹; Gennady Sukhikh¹; ¹Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, RUSSIA
- TP 102 **Using Mass Spectrometry to Identify IgG Fc and Fab Fragments Produced by Plasmin in Patient Serum**; David Barnidge¹; David Murray¹; ¹Mayo Clinic / DLMP, Rochester, MN
- TP 103 **Analysis of Sweat Volatiles using Solid Phase Microextraction in Conjunction with Gas Chromatography – Mass Spectrometry**; Courtney Weston¹; Changling Qiu¹; Kevin A. Schug¹; ¹The University of Texas, Arlington, TX
- TP 104 **Exploratory Study of NQO1 Expression in Advanced Solid Tumors**; Yuan Tian¹; Fabiola Cecchi¹; WEI-LI Liao¹; David E. Gerber²; David A. Boothman²; William Hoos³; Todd Hembrough¹; ¹Nantomics, Rockville, MD; ²University of Texas Southwestern Medical Center, Dallas, TX; ³NQ Oncology, INC, Chapel Hill, NC
- TP 105 **Quantification of MET by mass spectrometry for status assessment in prescreening of tumors for targeted therapies**; Kerry Scott¹; Fabiola Cecchi¹; Paolo Nuciforo²; Wei-Li Liao¹; ¹OncoPlex/NantOmics, Rockville, MD; ²Vall d'Hebron Institute of Oncology, Barcelona, Spain
- TP 106 **Approach to Implementing LC-MS/MS Plasma Metanephtrines : Calibrators, Sample Prep, Workflow**; Wai-Yoong Ng¹; Jinq Shya Yap²; Janelle SJ Chin²; Chin Pin Yeo²; ¹Singapore General Hospital, Singapore; ²Singapore General Hospital, Singapore, Singapore
- TP 107 **Identifications of Candidate Breast Cancer-Specific Biomarkers in Fresh Frozen Breast Tissue Sections by the MALDI-imaging Coupled with On-tissue Digestion**; Toyofumi Nakanishi; Osaka Medical College, Takatsuki, Japan
- TP 108 **Accurate Diagnosis for Prostate Cancer by Measuring the Ratio between Two Types of Prostate Specific Antigens by LDI-TOF MS**; Minyoung Yoo; Konkuk University, Seoul, South Korea
- TP 109 **LDTD-MS/MS Method for Quantitative Analysis of Four Immunosuppressant Drugs in Whole Blood and Cost Analysis Comparison to LC-MS/MS**; Stephen D Merrigan¹; Matthew Slawson²; Serge Auger³; Kamisha L Johnson-Davis^{1,4}; ¹ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; ²Utah Public Health Laboratory, Salt Lake City, UT; ³Phytronix Technologies, Quebec, QC; ⁴University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT
- TP 110 **Dried Blood Spots, Water-soluble Material and LC-MS based Protein Analysis**; Cecilie Rosting¹; Trine Grønhaug Halvorsen¹; Astrid Gjølstad¹; Christine Østvik Sævi¹; ¹School of Pharmacy, University of Oslo, Oslo, Norway
- TP 111 **The Impact of the Antigen-Antibody Interaction on the Tryptic Digestion in Immunocapture Based LC-MS/MS**; Maren Christin Stillesby Levernæs¹; Trine Grønhaug Halvorsen¹; Léon Reubsævi¹; Marianne Nordlund Broughton²; ¹School of Pharmacy, University of Oslo, Oslo, Norway; ²Radiumhospitalet, Oslo University Hospital, Oslo, Norway
- TP 112 **Analyte Sequestering Transport Particle Chromatography As A Front-End to Mass Spectrometry**; Fred Regnier¹; ZhiYu Li²; JinHee Kim²; ¹Purdue University / Novilytic, Carmel, IN; ²Novilytic, West Lafayette, IN
- DRUG DISCOVERY/DMPK/ADME (APPLICATIONS)**
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- TP 113 **Evaluation of the Pharmacokinetics of a Novel Anti-Diabetic Agent using Conventional LC/MS/MS**; Kenji Sugawara^{1,2}; Norihide Yokoi¹; Ritsuko Hoshikawa¹; Toshiya Matsubara³; Susumu Seino¹; ¹Division of Molecular and Metabolic Medicine, Kobe University Graduate School of Medicine, Kobe, Japan; ²Division of Diabetes and Endocrinology, Kobe University Graduate School of Medicine, Kobe, Japan; ³Shimadzu Corporation, Kyoto, Japan
- TP 114 **Quantification of Bindings of Organometallic Ruthenium Complexes to Protein Thiols by Mass Spectrometry**; Yumiao Han^{1,2}; Yu Lin¹; Fuyi Wang¹; ¹Institute of Chemistry Chinese Academy of Sciences, Beijing, China; ²University of Pennsylvania, Philadelphia, PA
- TP 115 **Proteome-wide drug dose-response of prostate cancer cell lines exposed to androgen receptor antagonists by microflow-LC SWATH MS analysis**; Ludovic Gillet¹; Sabine Amon¹; Yasuo Uchida¹; Nick Morrice²; Christie Hunter³; Ruedi Aebersold^{1,4}; ¹ETH Zurich, Zürich, Switzerland; ²SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA1 1RX; ³SCIEX, Redwood City, CA; ⁴University of Zurich, Zurich, Switzerland
- TP 116 **Peptide Metabolism: Identification of Metabolite Structures of GLP-1 Receptor Agonists in Different in vitro Systems Using High Resolution Mass Spectrometry**; Andreas Brink¹; Alessandra Piranha^{1,2}; Yves Siegrist¹; Aynur Ekiciler¹; Nicola Thum³; Fabien Fontaine⁴; Ismael Zamora⁴; Marcel Gubler¹; Silke Simon¹; Nicole Kratochwil¹; Simone Schadt¹; ¹Drug Disposition & Safety, Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland; ²Royal Melbourne Institute of Technology, Melbourne, Australia; ³School of Life Sciences, University of Applied Sciences and Arts Northwestern Switzerland, Basel, Switzerland; ⁴Lead Molecular Design, Sant Cugat de Valles, Spain
- TP 117 **Case Study of Stable-Isotopic Dilution for Accurate Mass Spectrometric Pharmacokinetic Quantitation of a Small Intact Protein from in vivo Samples**; Phillip Chu¹; Xinxin Gao¹; Susan Crowell¹; Leslie Dickmann¹; Rami Hannoush¹; Yichin Liu¹; John Tran¹; ¹Genentech Inc, South San Francisco, CA
- TP 118 **Metabolite Profiling and Covalent Binding of TAK-875 in Human Hepatocytes or Mitochondria**; Wing W Lam¹; Yong Gong¹; Rhys Salter¹; Mark R Player¹; David C Evans¹; Monicah Otieno¹; Heng-Keang Lim¹; ¹Janssen Research and Development, Spring House, PA
- TP 119 **High Resolution Accurate Mass Quantitation of Iloperidone and the Hydroxy Iloperidone Metabolite using Full Scan and Selected Ion Monitoring Modes**; David Brant¹; Keeley Murphy²; Jonathan L Josephs³; Maciej P Bromirski⁴; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher, San Jose, CA; ⁴Thermo Fisher Scientific, Bremen, DE
- TP 120 **Mechanism and Dynamics of SAMT Analog Inactivation of HIV-1 Gag Polyprotein**; Lisa M. Miller Jenkins¹; Elliott L Paine¹; Kara M. George Rosenker²; Harichandra D Tagad¹; Michael T Scerba²; Lalit Deshmukh²; Daniel H Appella²; ¹National Cancer Institute, NIH Bethesda, MD; ²National Institute of Diabetes and Digestive and Kidney Diseases, NIH, Bethesda, MD

- TP 121 **Development of a Magnetic Microbead Affinity Selection Screening with UHPLC-MS/MS for the Vitamin D Receptor**; Daniel Nosal¹; Michael D Rush¹; Jerry J White¹; Richard B van Breemen¹; ¹University of Illinois College of Pharmacy, Chicago, IL
- TP 122 **Implementation of Mass Spectrometry Ligand Binding (MS bind) Assays to Rapidly Identify Molecules for Radioligand Development for New Drug Targets**; Nathan G Hatcher¹; Rose B Flick¹; James W Monahan¹; Gary E Adamson¹; Nanyan Rena Zhang¹; Charles M Harrell¹; Victor N Uebele¹; ¹Merck & Co., Inc., West Point, PA
- TP 123 **Further Efforts towards Accurately Determining Unbound Fractions for Highly Plasma Protein Bound Compounds by LC-MS**; Inhou Chu; Merck & Co, Kenilworth, NJ
- TP 124 **In vitro Hepatic Metabolism of Licochalcone A, a Chalcone from the Licorice species Glycyrrhiza inflata.**; Lingyi Huang¹; Dejan Nikolic¹; Richard B. van Breemen¹; ¹University of Illinois College of Pharmacy, Chicago, IL
- TP 125 **Efficient and Cost-Effective In Vitro Permeability and Transporter Assessment Using the CACOReady 96-well Kit Assay and DiscoveryQuant 3.0**; Jeffrey Clarine¹; Katherine Andersen¹; Samuel Sperry¹; ¹eFFECTOR Therapeutics, San Diego, CA - California
- TP 126 **Effects of Intestinal Microbiota on the Bioavailability of Aspirin in Rats**; In Sook Kim; Shaheed Ur Rehman; Min Sun Choi; Jong Suk Park; Hyun Kim; Young Seok Ji; Hyeon Jun Kim; So Yeong Yun; ¹Hanyang University, Ansan-si, Gyeonggi-do
- TP 127 **A Validated Method for Anatabine Quantification in Human Plasma using High Resolution Parallel Reaction Monitoring Coupled with Chip-Based Nanospray**; Jon M Reed^{1,2}; Prashanthi Vallabhaneni²; Rosa Ajoy²; Gogce Crynen²; Laila Abdullah²; James E Evans²; Fiona Crawford¹; ¹SRQ Bio, Sarasota, FL; ²Roskamp Institute, Sarasota, FL
- TP 128 **A Multiplex Assay for Direct Analysis of Natural Products in Crude Botanical Extracts**; Geuncheol Gil¹; Pan Mao¹; Bharathi Avula²; Zulfiqar Ali²; Amar G. Chittiboyina²; Ikhlas A. Khan²; Larry A. Walker²; Daojing Wang¹; ¹Newomics Inc., Emeryville, CA; ²National Center for Natural Products Research, School of Pharmacy, The University of Mississippi, University, MS
- TP 129 **Recent Experience on LC-MS/MS Determination of ADC-like Drug Candidates and Corresponding Cytotoxic Agent in Biological Matrices**; Xiongfei Wu¹; Weimin Hu¹; Weiqun Cao¹; Yi Tao¹; Xinping Fang¹; Xin Zhang¹; ¹WuXi AppTec Co., Shanghai, China
- DRUG METABOLISM: QUALITATIVE AND HIGH THROUGHPUT ANALYSIS**
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- TP 130 **Development of an Automated High Throughput PAMPA Experiment for Permeability Assessment of Small Molecules and Peptides**; Xu Wang¹; Bernard K Choi²; Hui Wan²; Chen Shiyang²; Bahanu Habulihaz²; Gino M. Salituro²; Lucinda Cohen²; ¹Merck & Co., Rahway, NJ; ²Merck, Darmstadt, Germany
- TP 131 **Emerging Bioanalytical Tool to Characterize Drug and Drug-products of Biotherapeutics**; Jinal Patel¹; Mark Cancilla²; Xiang Yu²; Alina Dindyal-Popescu¹; Gordon Payne¹; Eva Duchoslav³; Suma Ramagiri⁴; ¹SCIEX, Concord, ON; ²Merck & Co., Inc., West Point, PA; ³SCIEX, Concord, ON; ⁴SCIEX, Concord ON, Canada
- TP 132 **Improved Data-Independent Workflow Strategies for Small Molecule Identification Using a High Resolution Q-TOF Mass Spectrometer**; Alina Dindyal-Popescu¹; Keith Goodman²; Eva Duchoslav³; Suma Ramagiri²; ¹SCIEX, Concord, ON; ²SCIEX, Concord ON, Canada; ³SCIEX, Concord, ON
- TP 133 **A Strategy for the Discovery and Identification of New Natural Product Metabolites by Orbitrap Mass Spectrometer and Multiple Data-Mining Approaches**; Chen Li¹; Ying Liu²; Jiayu Zhang²; Siyi Liu²; Wei Cai³; Jianqiu Lu²; ¹Thermo Fisher Scientific, Shanghai, China; ²Center of Scientific Experiment, Beijing University of Chinese Medicine, Beijing, China; ³Hunan University of Medicine, Huaihua, China
- TP 134 **Peptide Screening using Laser Desorption Ionization Mass Spectrometry on Fluorinated Nanopost Array (NAPA) Devices**; Trust Razunguzwa¹; Nicholas J Morris²; Heather Anderson²; Matthew J Powell²; Marvin S Yu³; ¹Protea Biosciences, Morgantown, WV; ²Protea Biosciences, Inc. Morgantown, WV; ³MS2 Array LLC, Pittsburgh, PA
- TP 135 **Metabolic Profiling of Two Novel Topo IIα Catalytic Inhibitors, Fluorescein Hydrazones in rat liver microsomes (RLMs) by LC-MS/MS**; Adnan A Kadi¹; Nasser S. Al-Shaklah¹; Youngjoo Kwon²; A. F. M. Motiur Rahman¹; ¹King Saud University, Riyadh-11451, Saudi Arabia; ²Ewha Womans University, Seoul, South Korea
- TP 136 **Metabolite Profile Comparison using a HµREL Co-culture Hepatocyte Model vs. a Conventional Hepatocyte Suspension for Low Turnover Drugs**; J. Matthew Hutzler¹; Richard D. Burton¹; Xiusheng Miao¹; Shelby Anderson¹; Todd Hieronymus¹; David Heim¹; Taysir Chamem¹; ¹Q2 Solutions, Indianapolis, IN
- TP 137 **Absorption, Distribution and Metabolism of Brodifacoum, a Potent Anticoagulant Rodenticide**; Zane Hauck¹; Douglas L Feinstein¹; Richard B van Breemen¹; ¹UIC, Chicago, IL
- TP 138 **Chiral Separation and Quantification of Metabolites using Super Critical Fluid Chromatography Coupled with Triple Quadrupole**; Siji Joseph¹; Syed S Lateef¹; ¹Agilent technologies, Bangalore, India
- TP 139 **In-vitro Synthesis of Drug Metabolites and Their Screening/Characterization Using Liquid Chromatography-Mass Spectrometry (LC-MS)**; Shubhashis Chakrabarty¹; Weilin L. L. Shelper¹; Andrew R. R. Thompson¹; David J. J. Smith¹; ¹USDA-Agricultural Research Service, Biosciences Research Laboratory, Fargo, ND
- TP 140 **Rapid Determination of Pharmacokinetic Profiles of Caffeine and Its Metabolites Collected on Skin by Ambient Mass Spectrometry**; Kun-Da Wu¹; Hung Su¹; Sychyi Cheng¹; JENTAIE SHIEA¹; ¹National Sun Yat-Sen University, Kaohsiung, TAIWAN
- TP 141 **Data Robustness of a High-Throughput Autosampler (Apricot Design Dual Arm-ADDA) in DiscoveryADME Sample Analysis**; Xiaotong Li¹; Yunqiang Su¹; Chunli Zhu¹; YI TAO²; Xinping Fang¹; Xin Zhang¹; ¹WuXi AppTec Co., Shanghai, China; ²WuXi AppTec Co., Shanghai, CHINA
- TP 142 **Dual-stream UHPLC Separations on a Compact Sample Delivery System Featuring Simplified Software Automation for Increased Throughput in Drug Discovery Bioanalysis**; John Janiszewski^{1,2}; Brendon Kapinos²; Wayne Lootsma³; Hui Zhang⁴; Julie keefe⁵; Steve Ainley³; Mary Piotrowski⁵; ¹Pfizer Inc., Groton, CT; ²Pfizer Worldwide Research and Development, Groton, CT; ³Sound Analytics, Niantic, CT; ⁴Pfizer Worldwide Research and Development, Inc Groton, CT; ⁵Pfizer, Groton, CT
- TP 143 **Determination of Heavy Metal Contamination in DMSO Solutions used for High Throughput Screening**; John M. Peltier¹; Nicole White²; Melissa Grippo¹; Jerome Giovanonni³; Pascal Bernet³; Christian Bergsdorf³; Justin Gu⁴; Zhaofu Wang⁴; Adam W Hill¹; ¹Novartis Institutes for Biomedical Research, Cambridge, MA; ²Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA; ³Novartis Institutes

- of BioMedical Research, Basel, Switzerland; ⁴Novartis Institutes of BioMedical Research, Shanghai, China
- TP 144 **Development of a Higher-throughput Metabolic Soft Spot Assay with Integrated Assessment of Glutathione Adduct Formation;** Anthony Paiva¹; Wilson Shou¹; Cheryl Klakouski¹; Tatyana Zvyaga¹; Benjamin Johnson¹; Yue-Zhong Shu²; Ismael Zamora³; ¹Bristol-Myers Squibb Company, Wallingford, CT; ²Bristol-Myers Squibb Company, Lawrenceville, NJ; ³Lead Molecular Design S.L., Sant Cugat de Valles, Spain

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- TP 145 **Photoionization as a Soft Ionization Source for Comprehensive Two-dimensional GC (GCxGC) and High-Resolution TOFMS;** Masaaki Ubukata¹; A. John Dane¹; Robert B. Cody¹; Toshiyuki Kato²; Masahiro Ito²; Bram van der Meer³; Junichi Osuga⁴; Jean-François Focant⁵; ¹JEOL USA, Inc., Peabody, MA; ²JEOL Ltd., Akishima, Japan; ³JEOL Europe B. V., Zaventem, Belgium; ⁴JEOL Europe SAS, Croissy-Sur-Seine, France; ⁵University of Liège, Liège, Belgium
- TP 146 **Investigation of the Partial Oxidation of Propane using a jet-Stirred Reactor and Molecular-Beam Mass Spectrometry;** Dennis Kaczmarek¹; Patrick Oßwald²; Dominik Krüger²; Markus Köhler²; Tina Kasper¹; ¹University of Duisburg-Essen, Duisburg, Germany; ²Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany
- TP 147 **Changing the Paradigm in Petroleomics with Comprehensive Two-Dimensional Gas Chromatography- High Resolution Mass Spectrometry;** Joe Binkley¹; Jonathan D Byer¹; David E Alonso¹; Lorne Fell¹; ¹LECO Corporation, Saint Joseph, MI
- TP 148 **Analysis of Petroleum Products using Comprehensive Two-Dimensional Gas Chromatography (GCxGC) with Both Time of Flight MS and Flame Ionization Detectors;** Christina Kelly¹; Joseph E Binkley¹; Lorne E Fell¹; Jonathan D Byer¹; David E Alonso¹; ¹LECO Corporation, Saint Joseph, MI
- TP 149 **A New Method for Characterizing Heavy Petrochemical Fractions Based on Thermal Analysis and Laser Photo Ionization Mass Spectrometry;** Ralf Zimmermann¹; Anne Ulbrich²; Thorsten Streibel³; Mohammad Saraji-Bozorgzad⁴; Sebastian Wohlfahrt³; Michael Fischer³; Thomas Denner⁵; Christoph Grimmer³; ¹University of Rostock, Rostock; ²University of Rostock, Rostock, N/A; ³University of Rostock, Rostock, Germany; ⁴Photonion GmbH, Schwerin, Germany; ⁵Netzsch Gerätebau GmbH, Selb, Germany
- TP 150 **Identification of the Byproducts in the Preparation of 2,6-naphthalenedicarboxylic Acid by UPLC-QTOF MS/MS;** Jiwen Li¹; Liyan Jiang²; Junyan Liu²; Chuan Wang²; ¹SINOPEC SRIPT, Shanghai, Shanghai; ²Sinopec Shanghai Research Institute of Petrochemic, Shanghai, China
- TP 151 **High Performance Thin Layer Chromatography (HPTLC) Coupled with DESI-Ion Mobility-Mass Spectrometry: A Novel Approach for Petroleum Characterisation;** Eleanor Riches¹; Caroline Mangote²; Delphine Thuault²; Pierre Giusti²; Carlos Afonso³; Peter Hancock¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²TOTAL Refining & Chemicals, Total Research & Technology Gonfreville, F-76700 Harfleur, France; ³Normandie Univ, COBRA, UMR6014 and FR3038, Université de Rouen; INSA de Rouen; CNRS, IRCOF, Rouen, France
- TP 152 **Intrinsic Ion Mobility Peak Width as an Indicator of Isomeric Species Distribution in Petroleum using Ion Mobility - Mass Spectrometry;** Mathilde Farenc^{1,2,3}; Eleanor Riches⁴; Carlos Afonso^{2,3}; Pierre Giusti^{1,3}; ¹TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; ²Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; ³TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, -, France; ⁴Waters, Wilmslow, United Kingdom
- TP 153 **Petroleomics by Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS);** Lilian Tose¹; Michael Murgu²; Boniek Gontijo Vaz³; Wanderson Romão¹; ¹UFES, Vitória, Brazil; ²waters Corporation, São Paulo, BRAZIL; ³UFG, Goiânia, Brazil
- TP 154 **Application of Paper Spray Ionization Mass Spectrometry for the Analysis of Weathered Oil;** Donghui Kim¹; Purum Kim²; Joon Geon An³; Un Hyuk Yim³; Sangwon Cha²; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, Republic of Korea; ²Hankuk Univ. Foreign Studies, Yongin, South Korea; ³Korea Institute of Ocean Science and Technology, Geoje, South Korea
- TP 155 **UnisprayTM Ion Source Coupled to UHPSFC for the Detection of Oilfield Additives;** Efstathios Andreas Elia¹; William Durnie²; Ed Sparke³; John G Langley¹; ¹Chemistry, University of Southampton, Southampton, United Kingdom; ²BP Exploration, Sunbury-on-Thames, Middlesex, United Kingdom; ³Waters, Wilmslow, United Kingdom
- TP 156 **Insights into Iron Promoted Sugar Conversion to 5-Hydroxymethylfurfural (HMF) and Levulinic Acid (LA) From Tandem Mass Spectrometry;** Yuan Jiang¹; Linan Yang¹; Christine M Bohn¹; Guannan Li¹; Dong Han¹; Nathan S Mosier¹; Jeffrey T Miller¹; Hilkka I Kenttämää¹; Mahdi M Abu-Omar¹; ¹Purdue University, West Lafayette, IN
- TP 157 **Untargeted Metabolomic Approach for the Management of Microbiologically Influenced Corrosion in the Oil and Gas Industry;** Vincent Bonifay¹; Iwona B Beech¹; Jan A Sunner¹; ¹University of Oklahoma, Norman, OK
- TP 158 **A Fast Mass Spectrometric Approach for the Characterization of Aromatic Compounds Present in Crude oil;** Ravikiran Yerabolu¹; Raghavendhar Kotha¹; Xueming Dong¹; John Kong¹; Bryan Clayton²; Hilkka Kenttämää¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Pioneer Oil Company, Lawrenceville, IL
- TP 159 **GC-MS and SFC-MS Approaches for the Low -level Detection and Quantification of a New Fuel Marker;** John G Langley¹; Julie M Herniman¹; Edward M. J. Wilmot¹; Anastarsia C. M. Carter¹; Jim Barker^{2,3}; ¹University of Southampton, Southampton, United Kingdom; ²Innospec Inc., Ellesmere Port, United Kingdom; ³Energy Institute, London, United Kingdom
- TP 160 **Comparison of GC-MS, GC-VUV, and Comprehensive Two-Dimensional GC for the Characterization and Source Identification of Diesel Fuels;** Ling Bai; ¹University of Texas at Arlington, Arlington, Texas
- TP 161 **Using GC/MSD with High Efficiency Source and Hydrogen Cleaning to Detect Low Level Contaminants in Ethylene and Propylene;** Angela Henry¹; Bruce Quimby¹; Badr Astiphan²; ¹Agilent Technologies, Little Falls, DE; ²Agilent Technologies, Santa Clara, CA
- TP 162 **Can Elusive Structural Features of Heavy Crude Oil Components be Decoded from FT-ICR-MS Data?;** Cristian Blanco-Tirado¹; Marianny Y Combariza²; Cristian Alejandro Blanco-Combariza²; ¹Universidad Industrial de Santander, Bucaramanga, Santander; ²Universidad Industrial de Santander, Bucaramanga, Santander, Colombia
- TP 163 **Highly Specific Biomarker Determination in Biodegraded Petroleum with Gas Chromatography and Triple Quadrupole Detection using Multiple Reaction Monitoring;** Andrés González¹; Taylor Motta¹; Ivama Calles¹; Sánchez Carlos¹; Jairo René Martínez¹; Stashenko Elena¹; ¹Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

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- TP 165 **Determination of Aqueous Film Forming Foam (AFFF) Components using a Multivariate Analysis Approach;** Lauren Mullin¹; Anna Karmann²; Gareth Cleland¹; John Vukovic¹; Adam Ladak¹; ¹Waters, Milford, MA; ²MTM Research Centre, Örebro University Örebro, Sweden
- TP 166 **Characterization of Fe-rich Multi-element Particles by ICP TOF;** Joel Kimmel¹; Olga Borovinskaya¹; Martin Tanner¹; ¹TOFWERK, Thun, Switzerland
- TP 167 **Polycyclic Aromatic Hydrocarbon and Metabolite Analysis of Soils Related to Energy Exploration by On-Line SFE/SFC-MS;** Doug D. Carlton^{1,2}; A. Paige Wicker¹; Kenichiro Tanaka³; Erin McAllister³; Kevin A Schug^{1,2}; ¹Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; ²Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX; ³Shimadzu Scientific Instruments, Inc., Columbia, MD
- TP 168 **Laser Desorption Single Particle Aerosol Mass Spectrometry for Direct Analysis of Solid Materials;** Mei Liu¹; Li Xu¹; Junguo Dong¹; Zhengxu Huang²; Ping Cheng³; Zhen Zhou²; ¹School of Environmental and Chemical Engineering, Shanghai University, Shanghai, China; ²Institute of Atmosphere environment security and Pollution control, Jinan University, Guangzhou, China; ³School of Environmental and Chemical Engineering, Shanghai University, Shanghai, Shanghai
- TP 169 **Development and Validation of a UPLC-MS/MS Method for Mono(2-ethylhexyl)phthalate, a Metabolite of Di(2-ethylhexyl)phthalate, in Rat Plasma, Amniotic Fluid, and Fetus;** Melanie A. Rehder Silinski¹; Brenda L. Fletcher²; Reshan A. Fernando²; Veronica G. Robinson³; Paul Foster³; Suramya Waidyanatha³; ¹RTI International, Research Triangle Park, NC; ²RTI International, Research Triangle Park, NC; ³Division of National Toxicology Program, NIEHS, Research Triangle Park, NC
- TP 170 **An Automated Method for Microcystins Analysis using Two-dimensional Liquid Chromatography-quadrupole Time-of-Flight Mass Spectrometry (2DLC-QTOFMS);** Xavier Ortiz Almirall¹; Marie Meyer-Monath²; Eva Korenkova¹; Karl Jobst¹; Eric Reiner¹; Karen MacPherson¹; ¹Ministry of the Environment and Climate Change of Ontario, Toronto, ON; ²University of Toronto, Toronto ON, Canada
- TP 171 **Development of an LC-QTOF MS Method for the Non-targeted Analysis of Microcystins;** Marie Meyer-Monath^{1,2}; Xavier Ortiz¹; Eva Korenkova¹; Ralph Ruffolo¹; Karl Jobst^{1,3}; Satyendra Bhavsar^{1,2,4}; Andre Simpson²; Eric Reiner^{1,2}; ¹Ontario Ministry of Environment & Climate Change, Toronto, Canada; ²University of Toronto, Toronto ON, Canada; ³McMaster University, Hamilton, Canada; ⁴University of Windsor, Windsor, Canada
- TP 172 **Determination of Trace Microcystins in Aqueous Samples by Solid-Supported Liquid Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry;** Chang-Lin Hsu¹; Chung-Yu Chen¹; Maw-Rong Lee²; ¹National Chung-Hsing University, Taichung, TAIWAN (R.O.C.); ²National Chung-Hsing University, Taichung, Taichung
- TP 173 **Effect of Analytical Standard Preparation Procedures in the Quantitation of Urinary Monohydroxy-Polycyclic Aromatic Hydrocarbons (OH-PAHs) by Online SPE-HPLC-MS/MS;** Yuesong Wang¹; Lei Meng¹; Erin N Pittman¹; Alisha Etheredge¹; Kendra Hubbard¹; Debra A Trinidad¹; Xiaoyun Ye¹; Antonia M. Calafat¹; ¹CDC, Atlanta, GA
- TP 174 **New 2,4-dinitroanisole (DNAN; Munitions Chemical) (bio)Transformation Products discovered and Bioassayed using High Resolution UPLC-QToFMS;** Leif Abrell¹; Christopher I. Olivares¹; Jon Chorover¹; Reyes Sierra-Alvarez¹; Jim A. Field¹; ¹University of Arizona, Tucson, Arizona
- TP 175 **Investigation of Eicosanoids and Fatty Acids in Pansteatitis-Affected Mozambique Tilapia at Loskop Dam, South Africa;** theresa cantu¹; John Bowden²; Jack McAlhany³; Matthew Guille⁴; hannes botha⁵; Louis J. Guille⁴; ¹MUSC, Charleston, SC; ²National Institute of Standards and Technology, Charleston, SC; ³college of charleston, charleston, SC; ⁴Medical Univ of S Carolina, Charleston, SC; ⁵Mpumalanga Tourism and Parks, Pretoria, South Africa
- TP 176 **Analysis of Problematic Cyclic Siloxane Compounds in the Atmosphere of the International Space Station;** Patti Cheng¹; Vanessa de Vera¹; Robert Gillispie¹; Steven Beck¹; William Wallace²; Thomas Limero²; ¹Wyle Science, Technology, and Engineering Group, Houston, TX; ², Houston, TX
- TP 177 **Accurate Mass Spectral Database: Harnessing the Power of High Performance Mass Spectrometry at Long Last;** Lorne Fell¹; Viatcheslav Artaev¹; Kevin McNitt¹; Steve Robles¹; Albert Lebedev²; ¹LECO Corporation, Saint Joseph, MI; ²Moscow State University, Moscow, Russian Federation
- TP 178 **A Method for Real-Time Monitoring of Acrolein in Air using TAGA Mass Spectrometry;** Nicholas Karelis; Ontario Ministry of the Environment, Toronto, ON
- TP 179 **Mass Spectrometry-based Studies on the Association of Organic Dusts and Respiratory Symptoms;** Brooke Thompson¹; Paulos Chumala¹; Shelley Kirychuk¹; George S. Katselis¹; ¹CCHSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada
- TP 180 **Monitoring Fugitive Emissions with a Miniature Ion Trap Mass Spectrometer;** Preshious Rearden¹; Corey Stedwell¹; Parminder Kaur¹; Daniel DeBord¹; ¹1st Detect Corporation, Webster, TX
- TP 181 **Analytical Strategy to Investigate Naphthenic Acids in Atmospheric Aerosols by Ultrahigh-Performance Liquid Chromatography-quadrupole Time-of-Flight Mass Spectrometry (UPLC/QTOF-MS);** Mahmoud Yassine; Environment and Climate Change Canada, Ottawa, ON
- TP 182 **A Comparison of Thermal- and Valve-based Modulation for the Analysis of Environmental Contaminants by GCxGC-TOF MS;** Tadeusz Gorecki¹; Matthew Edwards^{1,2}; Haleigh Boswell¹; Pete Grosshans³; ¹University of Waterloo, Ontario, Canada; ²Markes International, Cardiff, UK; ³Markes International Inc, Cincinnati, OH
- TP 183 **High sensitive quantitation method of perfluorinated compounds by an automated online solid extraction LC/MS/MS;** Yoshikane Mitsuha¹; Jun Watanabe²; Kagi Noriko³; Minohata Toshikazu⁴; Ogura Tairo⁵; Nakayama Shoji⁶; ¹IDEA Consultants, Inc., Yaidzu, Japan; ²Shimadzu Corporation, Kyoto; ³JASCO International Co., Ltd., Hachioji, Japan; ⁴Shimadzu Corporation, Kyoto, Japan; ⁵Shimadzu Scientific Instruments, Inc. Columbia.; ⁶National Institute for Environmental Studies, Tsukuba, Japan
- TP 184 **A Collaborative EPA Method 625 Update Study using a New Mass Spectrometry Method for Quantification Combined with Stir-bar Sorptive Extraction;** Weier Hao¹; Andrew Boggess¹; Edward Pfannkuch²; Skip Kingston¹; ¹Duquesne University, Pittsburgh, PA; ²Gerstel, Inc. Linthicum, MD

- TP 185 **Automated Screening of Explosives in Soil Samples by Online SFE-SFC-MS**; William A Hedgepeth¹; Kenichiro Tanaka²; Tairo Ogura²; Jonathan Edwardsen²; ¹Shimadzu Scientific Instruments, Inc, Columbia, MD; ²Shimadzu Scientific Instruments, Inc, Columbia, MD
- TP 186 **Efficiency Screening of Carbon Nanomaterial or Superoxydant in Advanced Water Treatment by Mass Spectrometry Are They Accurate Enough?**; Hugues Preud'homme¹; Jaber Al-Marri¹; Pierre Kubiak¹; Rachid Essehli¹; ¹QEERI - HBKU - Qatar Foundation, Doha, QATAR
- TP 187 **Chromatographic Mass Spectrometric Detection of Arsenic Species in Sulfidic Waters – Method Development**; Denzel Bolden¹; Akeena Harper¹; Jianye Zhang¹; ¹Voorhees College, Denmark, SC
- TP 188 **Fast Detection of Environmental Vapors by Thermal Desorption - Atmospheric Pressure Photoionization - Differential Mobility Analysis - Mass Spectrometry (TD-APPI-DMA-MS)**; Ross David McCulloch¹; Amo González Mario¹; ¹SEADM, Boecillo, Spain

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- TP 190 **Resolution of Isotopologues and Isotopomers by High-Field Ion Mobility Coupled to Mass Spectrometry: Path to Gas-Phase NMR?**; Julia Kaszycki¹; Matthew A. Baird¹; Andrew P. Bowman¹; Alexandre A Shvartsburg¹; ¹Wichita State University, Wichita, KS
- TP 191 **Modeling and Characterization of the Ion Transit Time in a FAIMS-MS Interface**; Satendra Prasad¹; Jean-Jacques Dunyach¹; Michael W Belford¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 192 **On a Multi-physics Computational Model to Understand Heat Exchange between FAIMS Electrode and Ion Transport Gas**; Satendra Prasad; ¹Thermo Fisher Scientific, San Jose, CA
- TP 193 **Efficiency of Ion Transmission between FAIMS Electrodes without a Separation Electric Field**; Satendra Prasad¹; Susan E Abbatiello²; Michael W Belford¹; Jean-Jacques Dunyach¹; Mary L Blackburn¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Cambridge, USA
- TP 194 **Comparison of Rectangular Waveform FAIMS/MS to Conventional Sum-of-sines Waveform**; Michael Wei¹; Michael Costanzo¹; Joaquin Casanova¹; Jared Boock¹; Richard A Yost¹; ¹University of Florida, Gainesville, Florida
- TP 195 **Glyphosate quantified in Black Tea and Other Food Matrices by Automatically Optimized LC-FAIMS MS/MS**; Bennett Kalafut¹; Rae Ana Snyder¹; Claudia Martins¹; Manish Doshi¹; Mark Hardman¹; ¹Thermo Fisher Scientific, San Jose, California
- TP 196 **Rapid FAIMS at Extreme Fields Inside the Mass Spectrometry Envelope with Applications to Peptide and Protein Analyses**; Alexandre Shvartsburg¹; Andrew Entwistle²; Roger Giles²; ¹Wichita State University, Wichita, KS; ²Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom
- TP 197 **Is Differential Mobility Chemically Driven? Evidence and Simulations for Chemical Effects as Primary Separation Factor in DMS**; Walter Wissdorf¹; Bradley B Schneider²; Tom Covey²; James Hager²; Thorsten Benter³; ¹Bergische Universität Wuppertal, Wuppertal; ²SCIEX, Concord, ON; ³Bergische Universität Wuppertal, Wuppertal, Germany
- TP 198 **LESA FAIMS Mass Spectrometry for the Spatial Profiling of Proteins from Tissue**; Rian L. Griffiths¹; Alex Dexter¹; Andrew J Creese¹; Alan M. Race²; Josephine Bunch^{2,3}; Helen Cooper¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, Teddington, UK; ³University of Nottingham, Nottingham, UK
- TP 199 **Analysis of Derivatized Glycans using Differential Mobility Spectrometry**; Cathy Lane¹; Yves J C LeBlanc²; J. Larry Campbell²; ¹SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA1 1RX; ²SCIEX, Concord, ON
- TP 200 **Improved Quantitative Measurements for Large Scale Proteomic Analyses using Metabolic Labeling and Ion Mobility**; Sibylle Pfammatter¹; Eric Bonnell²; Pierre Thibault¹; ¹IRIC-Université de Montréal, Montréal, QC; ²Université de montréal, Montreal, QC
- TP 201 **Model FAIMS RF System using Neural Network**; Xiaoqun Zou; ¹ThermoFisher Scientific, San Jose, CA
- TP 202 **Making FAIMS Faster, More Selective, and More Sensitive**; Michael Belford¹; Satendra Prasad¹; Jean-Jacques Dunyach¹; Susan E Abbatiello¹; Ryan Hermezian¹; Hoa Pham¹; Ann Yadowsky¹; Alex Zou¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 203 **Selextion-based Detergent Interference Removal for Shotgun-Lipidomics Analyses**; Cyrus Papan¹; Julian D Langer²; ¹Sciex, Darmstadt, Hessen; ²Max-Planck-Institute of Biophysics, Frankfurt Am Main, Germany
- TP 204 **Rapid Analysis of Steroid Metabolites using Field Asymmetric Waveform Ion Mobility Spectrometry Combined with Liquid Chromatography and Mass Spectrometry**; Kayleigh Louise Arthur¹; Matthew Arran Turner¹; James Christopher Reynolds¹; Colin Creaser¹; ¹Loughborough University, Loughborough, United Kingdom
- TP 205 **Differential Mobility Spectrometry (DMS) Reveals the Elevation of Urinary Acetylcarnitine in Non-Human Primates (NHP) Exposed to Radiation**; Nicholas B. Vera^{1,2}; Amol Kafle³; Evan Pannkuk⁴; Evagelia C. Laiakis⁴; A.J. Fornace, Jr.⁴; Stephen L. Coy³; Derek M Erion¹; Paul Vouras³; ¹Pfizer, Cambridge, MA; ²Northeastern University, Boston, Massachusetts; ³Northeastern University, Boston, MA; ⁴Georgetown University, Washington, DC
- TP 206 **Characterization of Variables Affecting Internal Energy Deposition inside a Differential Ion Mobility Spectrometer**; Brandon Santiago¹; Matthew T. Campbell¹; Gary L. Glish¹; ¹The University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 207 **Analysis of Free Drug in Antibody-Drug Conjugate by Reversed-phase HPLC Coupled with Differential Mobility Mass Spectrometry**; Chunang (Christine) Gu¹; Marie-France Morissette²; Loren Y Olson³; Shaokun Pang³; Yi Li²; Colin Medley²; David Russell²; ¹Genentech, South San Francisco, CA; ²Genentech Inc, South San Francisco, CA; ³SCIEX, Redwood City, CA
- TP 208 **Optimizing DMS Separations by Comparing Alpha Functions**; Brad Schneider¹; Erkinjon Nazarov¹; J.C. Yves Le Blanc¹; Frank Londry¹; Thomas Covey¹; ¹SCIEX, Concord ON, Canada
- TP 209 **Rapid Ion Trap Mass Analysis of Inorganic Water Clusters Separated by Differential Mobility Spectrometry**; Theresa Evans-Nguyen¹; Timothy Vazquez¹; ¹University of South Florida, Tampa, FL

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- TP 212 **GC/MS/MS Analysis of Pesticide Residues in Cannabis Using QuEChERS Extraction and Cleanup**; Kathy Stenerson¹; Craig Aurand¹; David Bell¹; Sara Smith¹; Emily Barrey¹; Candace Price¹; ¹MilliporeSigma, Bellefonte, PA
- TP 213 **Analysis of Pesticides in Spaghetti Sauce by Direct Immersion Solid Phase Microextraction GC/MS**; Kathy Stenerson¹; Candace Price¹; Craig Aurand¹; Dave Bell¹; Emily Barrey¹; Sara Smith¹; ¹Sigma Aldrich, Bellefonte, PA
- TP 214 **An Optimal Method for the Analysis of Pesticides in a Variety of Matrices**; Jessica Westland¹; Vivian Chen²; ¹Agilent Technologies, Wilmington, Delaware; ²AGILENT, Shanghai, China
- TP 215 **Accurately Identify and Quantify A Hundred Pesticides in a Single GC Run**; Jessica Westland¹; Tom Doherty²; Vivian Chen³; ¹Agilent Technologies, Wilmington, Delaware; ²Agilent Technologies, Santa Clara, CA; ³Agilent, Shanghai, China
- TP 216 **Maintaining Sensitivity and Reproducibility with the Self Cleaning Ion Source for Pesticides in Food and Feed**; Vivian Chen¹; Jessica Westland²; Elizabeth Almasi³; ¹Agilent, Shanghai, China; ²Agilent Technologies, Wilmington, Delaware; ³Agilent Technologies, Santa Clara, CA
- TP 217 **"No Dilute" Just Shoot LC-ESI-MS/MS : Feasibility and Robustness of a Maintenance-Free Source for Applications in Low-level Pesticide Residue Analysis**; Matteo Meglioli¹; Frank A Kero²; Joshua Ye³; Craig Young²; Sharanya Reddy²; ¹Mosti Mondiale, Villa Ste Catherine, QC; ²PerkinElmer, Shelton, CT; ³Ionics Mass Spectrometry Group, Bolton, ON
- TP 218 **Rapid Detection of Pesticides in Honey by C18 Pipette-tip Electrospray Ionization Mass Spectrometry**; Yi-Ching Choi¹; Tsz-Tsun Ng¹; Bin Hu¹; Zhong-Ping Yao¹; ¹Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China
- TP 219 **A Single LC-MS/MS Method for Confirmation and Quantification of over 400 Pesticides in Complex Matrix without Compromising Data Quality**; Dimple Shah¹; Eimear McCall²; Gareth Cleland³; ¹Waters Corp., Milford, MA; ²Waters, Wilmslow, United Kingdom; ³Waters Corporation, Milford, MA
- TP 220 **Determination of Multiple Pesticides Residues in Imported Tea in UAE Using Liquid and Gas Chromatography Tandem Mass Spectrometry**; Mohammed Meetani¹; Sarah Ali Almulla^{2,3}; Nasra M. Ibrahim²; ¹United Arab Emirates University, Al-Ain, Abu Dhabi; ²laboratories Department, Ministry of Environment and Water, Sharjah, United Arab Emirates; ³chemistry Department, College of Science, UAE University, Al-Ain, United Arab Emirates
- TP 221 **Multi-residue Analysis of Pesticides in Agricultural Products using QuEChERS and SFC/MS**; Yuka Fujito¹; Kenichiro Tanaka²; Tairo Ogura²; Kiyomi Arakawa¹; Yoshihiro Hayakawa¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instruments, Inc. Columbia
- TP 222 **Supercritical Fluid Chromatography/Tandem Mass Spectrometry (SFC-MS/MS) Analysis of Hundreds of Pesticide Residues in Food Safety**; David Baker¹; Christopher Titman¹; Jonathan Horner²; Neil Loftus¹; ¹Shimadzu, Manchester, UK; ²SAL (Scientific Analysis Laboratories), Cambridge, UK
- TP 223 **Quantitative Analysis of 647 Pesticides (1,929 MRMs) by LC-MS/MS with a Fast 10.5 Minute Cycle Time**; David Baker¹; Laetitia Fages²; Eric Capodanno²; Neil Loftus¹; Simon Ashton¹; ¹Shimadzu, Manchester, UK; ²Phytocontrol, Nimes, France
- TP 224 **Food Residue Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) - Multi-Pesticide Identification and Quantitation**; KC Hyland¹; Paul Winkler¹; Andre Schreiber²; ¹SCIEX, Redwood City, CA; ²AB SCIEX, Concord, ON
- TP 225 **Screening of Pesticides in Lipid-rich Food Matrices by using High Resolution GC/Q-TOF and Accurate Mass Pesticide Library**; Kai Chen¹; Joan Stevens²; Hong Chen¹; Vadim Kalmeyer¹; Sofia Nieto¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Wilmington, DE
- TP 226 **Routine Quantitative and Qualitative Methodologies for Food Pesticide Residue Laboratories Using Tandem and High Resolution Accurate Mass (HRAM) LC/MS Instrumentation**; Claudia Martins¹; Ed George¹; Dipankar Ghosh¹; Katerina Bousova²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Dreieich, Germany
- TP 227 **Screening for More than 600 Pesticide Residues and Their Identification in Food Samples using a New LCMSMS Library Data Base**; Houssain El Aribi¹; Salah A. Almaman¹; Mustafa A. Gassem¹; Majed A. Alansari¹; ¹Saudi FDA, Riyadh
- TP 228 **Rapid Extraction and Clean-up Kits for the Determination of Pesticide Residues in Food**; Shao Kai Lin; Taichung, Taichung
- TP 229 **Development of Multi-Pesticides in Avocado using Enhanced Matrix Removal by liquid Chromatography-Tandem Mass Spectrometry with Dynamic MRM and Triggered MRM**; Wen-Yen Lee¹; Jin-Lan Sun²; Chun-Ye Sun²; Shan-An Chan¹; ¹Agilent, Taipei, Taiwan; ²Agilent, Shanghai, China
- TP 230 **Rapid Screening and Quantitation of Pesticide Residues in Cannabis by Modified QuEChERS and LC-MS-MS**; Jeff Dahl¹; Julie Kowalski²; Gordon Fagras³; ¹Shimadzu, Columbia, MD; ²Restek Corporation, Bellefonte, PA; ³Trace Analytics, Spokane, WA
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- TP 232 **Fast Data Acquisition Speed and High quantitative Performance in the Simultaneous Determination of Mycotoxins, Illegal Dyes and Pesticides in Spices**; Mark Sartain¹; Thomas Glauner²; Craig Marvin³; Andre Santos⁴; Anumol Tarun³; Jerry Zweigenbaum³; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; ³Agilent Technologies, Wilmington, DE; ⁴Agilent Technologies Inc, Barueri, Brazil
- TP 233 **Multi-Residue Pesticides Analysis by LC-MS/MS using the ODS Column and the Biphenyl Column**; Natsuyo Asano¹; David Baker²; Yuki Uno¹; Atsuhiko Toyama¹; Jun Watanabe¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu, Manchester, UK
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- TP 239 **The Modernisation of Fish Fraud Detection using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)**; Connor Black¹; Olivier Chevallier¹; Julia Balog²; Sara Stead³; Steven D Pringle⁴; Christopher Elliott¹; Zoltan Takats⁵; ¹Queens University Belfast, Belfast, UK; ²Waters WRC, Budapest, Hungary; ³Waters corp, Manchester, Lanc; ⁴Waters, Wilmslow, United Kingdom; ⁵Imperial College, London, United Kingdom
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- TP 245 **Analysis of Pinot Noir Wines by HS-SPME GC/Q-TOF: Correlating Geographical Origin with Volatile Aroma Profiles**; Philip L. Wylie¹; Anna K. Hjelmeland²; Ron C. Runnebaum²; Susan E. Ebeler²; ¹Agilent Technologies, Wilmington, DE; ²University of California-Davis, Davis, CA
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- TP 250 **Analysis of the Oligosaccharide and Protein Content of Beer Using Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry (MALDI TOFMS)**; Elsa Gorre¹; Ashley Phetsanthad¹; Jon Soffer¹; Kevin G Owens¹; ¹Drexel University, Philadelphia, PA
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- TP 254 **Forensic Identification of Unknown Compounds in Human Urine Using Complimentary Software with High-Resolution Data and Theoretical Fragmentation Spectra**; Kristine Van Natta¹; Marta Kozak¹; Xiaolei Xie¹; Mindy Gao¹; ¹Thermo Fisher Scientific, San Jose, CA
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- TP 267 **Protein Profiling of Decedent Scalp Hair Segments Exhibiting a Post-Mortem Hair Root Band**; McKay B. Allred¹; Brian A. Eckenrode¹; Traci L. Carlson¹; Jamie N. Fleming¹; Nicholas R. Vercruyssen¹; Andrew W. Plotner¹; Hilda S. Castillo¹; Dawnie W. Steadman²; Lee M. Jantz²; Kathleen Hauther²; Jack Hietpas¹; JoAnn Buscaglia¹; Stephen D. Shaw¹; Mehdi Moini³; Joseph Donfack¹; ¹FBI Laboratory, Quantico, VA; ²University of Tennessee, Knoxville, TN; ³George Washington University, Washington DC
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- ⁴; Cesare Galli^{5, 6, 7}; Andrea Perota⁵; Sophie Conchon⁸; Jean-Paul Concordet⁸; Jean-Paul Judor⁸; Giovanna Lazzari^{6, 7}; Jean-Paul Souillou⁸; Helene Perreault¹; ¹University of Manitoba, Winnipeg, MB; ²Xenothera, Nantes, France; ³Massachusetts General Hospital, Boston, MA; ⁴Harvard Medical School, Boston, MA; ⁵Avantea Laboratorio Di Tecnologie Della Riproduzione, Cremona, Italy; ⁶Fondazione Avantea, Cremona, Italy; ⁷University of Bologna, Bologna, Italy; ⁸Université de Nantes, Nantes, France; ⁹Université de Paris-Descartes, Paris, France
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- TP 298 **Optimisation of Two-Dimensional FT-ICR MS for IR-ECD**; Maria Van Agthoven¹; Federico Floris²; Alice Lynch²; Christopher Wootton²; Lionel Chiron³; Mark P Barrow²; Marc-André Delsuc⁴; Christian Rolando⁵; Peter B O'Connor²; ¹University of Warwick, Coventry, Midlands; ²University of Warwick, Coventry, United Kingdom; ³CASC4DE, Strasbourg, France; ⁴IGBMC, Illkirch-Graffenstaden, France; ⁵Université Lille 1, Sciences et Technologies Villeneuve d'Ascq, France
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- TP 300 **Mass Defect-based N,N-Dimethyl Leucine (DiLeu) Labels for quantitative Proteomics and Amine Metabolomics of Pancreatic Cancer Cells**; Ling Hao¹; Jillian Johnson²; Christopher Lietz²; W. John Kao²; Lingjun Li²; ¹University of Wisconsin Madison, madison, WI; ²University of Wisconsin-Madison, Madison, WI

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- TP 306 **Implementation of the All Ion Fragmentation Analysis for Targeted/Untargeted Metabolomic Approaches**; Enrique Sentandreu¹; Shannon R Sweeney¹; Jennifer Chiotu¹; Stefano Tiziani¹; ¹Dell Pediatric Research Institute, Austin, Tx
- TP 307 **Accurate FT-ICR MS with Fluctuating Ion Sources**; Konstantin O Nagornov¹; Anton N Kozhinov¹; Yuri O Tsybin¹; ¹Spectroswiss Sàrl, Lausanne, Switzerland
- TP 308 **Characterization of a Modified Dynamically Harmonized FT-ICR Cell at High Magnetic Field**; Christopher L Hendrickson^{1,2}; Nathan K Kaiser¹; Steven C Beu³; Greg T Blakney¹; John P Quinn¹; Donald J Smith¹; Alan G Marshall^{1,2}; ¹Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; ²Department of Chemistry, Florida State University Tallahassee, FL; ³S C Beu Consulting, Austin, TX
- TP 309 **Boosting FTMS Performance via Advanced Data Acquisition Electronics and Signal Processing**; Yury O Tsybin¹; Konstantin O Nagornov¹; Anton N Kozhinov¹; ¹Spectroswiss Sàrl, Lausanne, Switzerland
- TP 310 **Implementation of a High-performance FPGA-based Data Acquisition System for FTMS**; Anton Kozhinov¹; Konstantin Nagornov¹; Yuri Tsybin¹; ¹Spectroswiss Sàrl, Lausanne, Switzerland
- TP 311 **Design of Automated Quantitative Optimization Software for Hi-Resolution Analysis**; Eugene F. Ciccimaro¹; Asoka Ranasinghe²; Timothy Olah²; Richard Baran³; Mark Sanders³; Jonathan L Josephs³; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Princeton, NJ; ³Thermo Fisher Scientific, San Jose, CA
- TP 312 **9-plex Metabolic Labeling with NeuCode SILAC**; Katherine A Overmyer¹; Elyse C Freiburger¹; Stefka Tyanova²; Anna E Merrill¹; William Wood³; Marwan Elmasri³; Alexander S Hebert¹; Michael S Westphall¹; Joel C Bradley³; Juergen H Cox²; Joshua J Coon¹; ¹University of Wisconsin Madison, Madison, WI; ²Max Planck Institute of Biochemistry, Martinsried, DE; ³Cambridge Isotope Laboratories, Inc. Tewksbury, MA
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- TP 313 **New Insights into the Microenvironment of Cancerous Tissue by Combined Mass Spectrometry, Microscopy and Multivariate Analysis**; Tina Angerer¹; John Stephen Fletcher¹; ¹University of Gothenburg, Gothenburg, Sweden
- TP 314 **Typing of Colon and Lung Adenocarcinoma using High-throughput Imaging Mass Spectrometry**; Rita Casadonte¹; Mark Kriegsmann²; Rémi Longuespée¹; Petra Wandernoth^{1,3}; Cristina Mohanu³; Tiemo Katzenberger⁴; Daniela Aust⁵; Gustavo Baretton⁵; Jörg Kriegsmann^{1,3,6}; ¹Proteopath GmbH, Trier, Germany; ²University of Heidelberg, Heidelberg, Germany; ³Molekularpathologie Trier, Trier, Germany; ⁴Department of Pathology, Hospital Aschaffenburg, Aschaffenburg, Germany; ⁵University of Dresden, Dresden, Germany; ⁶Center for Histology, Cytology and Molecular Diagnostics Trier, Trier, Germany
- TP 315 **Desorption Electrospray Ionisation Imaging towards Enhanced Breast Cancer Diagnosis**; Dipa Gurung¹; James McKenzie¹; Francesca Rosini¹; Luisa Doria¹; Anna Mroz¹; Rathi Ramakrishnan¹; Edward R St John¹; Jeremy K Nicholson¹; Zoltan Takats¹; ¹Imperial College London, South Kensington Campus London, United Kingdom
- TP 316 **MALDI-MS Imaging of Lipid Changes after PI3-K Inhibition in Colorectal Cancer Liver Metastases**; Fiona Henderson¹; Irma Berrueta Razo²; Nicholas Lockyer²; Omar Belgacem³; Kaye J Williams⁴; Adam McMahon¹; ¹Wolfson Molecular Imaging Centre, University of Manchester, Manchester, England; ²Manchester Institute of Biotechnology, University of Manchester, Manchester, England; ³Shimadzu, Manchester, England; ⁴Stopford Building, University of Manchester, Manchester, England
- TP 317 **Multimodal imaging of lipids in a Zebrafish Melanoma Model by PET and DESI-MS**; Emrys Jones¹; Fiona Henderson²; Anthony Midey³; Adam Hurlstone²; Duncan Foster²; Hannah Johnston²; Kaye Williams²; Adam W McMahon²; Emmanuelle Claude¹; ¹Waters Corporation, Wilmslow, UK; ²Wolfson Molecular Imaging Centre, Manchester, UK; ³Waters Corporation, Beverly, Massachusetts
- TP 318 **Comparative Mapping of PSA and N-glycan Distributions in FFPE Prostate Cancer Tissues using MALDI-FTICR and Rapid MALDI-TOF Mass Spectrometry Imaging**; Richard R Drake¹; Peggi M Angel¹; Hendrik Jan Kobarg²; Shannon Cornett³; ¹Medical University of South Carolina, Charleston, SC; ²SCILS GmbH, Bremen, Germany; ³Bruker Daltonik, Billerica, MA
- TP 319 **Imaging Mass Spectrometry Approach for the Diagnosis of Carcinoma of the Cervix**; Rita Casadonte¹; Rémi Longuespée¹; Mark Kriegsmann²; Michael Becker³; Sören-Oliver Deininger³; Mike Otto¹; Jörg Kriegsmann^{1,4}; ¹Proteopath GmbH, Trier, Germany; ²University of Heidelberg, Heidelberg, Germany; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany



- TP 320 **MALDI Imaging a Tool for Clinical Diagnostic – Classification of Prostate Cancer Subgroups;** Birte Beine¹; Tobias Boskamp²; Dimo Dietrich³; Hendrik Jan Kobarg⁴; Konrad Steinestel⁵; Piotr Widlak⁶; Barbara Sitek⁷; Helmut Erich Meyer⁸; Corinna Henkel⁹; ¹ISAS e.V., Dortmund, NRW; ²Center for Industrial Mathematics, University of Bremen, Bremen, Germany; ³Institute of Pathology, University Hospital Bonn (AöR), Bonn, Germany; ⁴SCILS GmbH, Bremen, Germany; ⁵Gerhard-Domagk-Institute of Pathology, University Hospital Münster (UKM), Münster, Germany; ⁶Center for Translational Research and Molecular Biology of Cancer, Maria Skłodowska - Curie Memorial Cancer Center and Institute of Oncology, Gliwice, Poland; ⁷Medizinisches Proteom-Center, Ruhr-Universität Bochum, Bochum, Germany; ⁸ISAS - e.V., Dortmund, Germany
- TP 321 **Molecular Markers of Serous Ovarian Cancer Aggressiveness and Surgical Outcome by Ambient Ionization Mass Spectrometry Imaging;** Marta Sans Escofet¹; Kshipra Gharpure²; Jialing Zhang¹; Jinsong Liu²; Anil K. Sood²; Livia S. Eberlin¹; ¹University of Texas at Austin, Austin, TX; ²the University of Texas M.D Anderson Cancer Center, Houston, TX
- TP 322 **Linking Lipid Metabolism, Hypoxia, Radiation Therapy and Metastasis using DESI Imaging Mass Spectrometry;** Erik J. Soderblom¹; Kathleen Ashcraft²; Matt W. Foster³; Emmanuelle Claude⁴; Emrys A Jones⁴; James Langridge⁴; M. Arthur Moseley³; Mark Dewhirst²; ¹Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham, NC; ²Radiation Oncology, Duke University Medical Center, Durham, NC; ³Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham, NC; ⁴Health Sciences, Waters Corp, Manchester, UK
- TP 323 **Elemental Analysis and Imaging of Stroke-affected Brain Tissues by Utilizing Laser Ablation-inductively Coupled Plasma-Mass Spectrometry: Diagnostic Study;** Khalid A. Al-Saad¹; Mohamed H Ali²; MD Fazle Rakib¹; Eman M Fayyad¹; Rick Dijkhuizen³; Geralda V Tilborg⁴; ¹Qatar University, Doha, Doha; ²Qatar Biomedical Research Institute, Doha, Qatar; ³University Medical Center Utrecht, Utrecht, Netherlands
- TP 324 **Molecular Signature Discovery of Human Chronic Traumatic Encephalopathy Tissues using Mass Spectrometry Imaging;** Bo Yan¹; Dharmendra B. Goswami¹; Deborah R Leon¹; Mark E McComb¹; Ann C. McKee^{1,2}; Catherine E Costello¹; ¹Boston University School of Medicine, Boston, MA; ²United States Department of Veterans Affairs, VA Boston Healthcare System, Boston, MA
- TP 325 **MALDI Imaging of Neuronal Plasticity: Analysing Fine Adaptations with Large Effects;** Jakob Meier-Credo¹; Michael Becker²; Alice Ly²; Shahar Or¹; Irina Epstein¹; Thomas Hagedorn²; Tamas Dalmay¹; Johannes J Letzkus¹; Erin Schuman¹; Julian Langer¹; ¹Max-Planck-Institute for Brain Research, Frankfurt Am Main, Germany; ²Bruker Daltonik GmbH, Bremen, Germany
- TP 326 **Nanoparticle Matrix Implantation Mass Spectrometry Imaging Discovers and Quantifies Lipid Biomarkers of Traumatic Brain Injury and Tracks Therapeutic Response;** Aurelie Roux¹; Ludovic Muller²; Shelley N Jackson²; Jeremy Post; Katherine Baldwin³; Barry Hoffer⁴; Carey Balaban⁵; Damon Barbacci⁶; Albert J Schultz⁷; Shawn Gouty⁸; Brian M Cox⁸; Amina S Woods⁹; ¹All Children's Hospital Johns Hopkins Medicine, Saint Petersburg, FL; ²NIH/NIDA-IRP, Baltimore, MD; ³Philadelphia College of Osteopathic Medicine, Philadelphia, PA; ⁴University Hospitals of Cleveland, Cleveland, OH; ⁵University of Pittsburgh, Pittsburgh, PA; ⁶Ionwerks, Gaithersburg, MD; ⁷Ionwerks Inc, Houston, TX; ⁸Uniformed Services University, Bethesda, MD; ⁹NIDA-IRP, NIH Baltimore, MD
- TP 327 **MALDI Mass Spectrometry Imaging in Alzheimer's disease mouse model Het CRND8 (+/-);** Lyna Sellami¹; Marcia Roy²; Matthew E Openshaw¹; Luis Mancera¹; Omar Belgacem¹; ¹Shimadzu, Kratos Manchester, United Kingdom; ²University of Edinburgh, Edinburgh, UK
- TP 328 **Simultaneous MALDI MS Imaging and Quantitation of Multiple Neurotransmitters in Parkinson's Disease Models;** Elva Fridjonsdottir¹; Mohammadreza Shariatgorji¹; Anna Nilsson¹; Patrik Källback¹; Xiaoqun Zhang²; Per Svenningsson²; Per E. Andren³; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institutet, Stockholm, Sweden; ³Uppsala University, Uppsala, SE
- TP 329 **Detection of Ganglioside Lipid Species in the Brain of Mucopolysaccharidosis Type II Mouse by Imaging Mass Spectrometry;** Martin Dufresne¹; Daniel Guneyusu¹; Martin Marcinkiewicz²; Anthony Regina³; Michel Demeule³; Pierre Chaurand⁴; ¹Université de Montréal, St-Hyacinthe, QC; ²Cytochem Inc., Montreal Quebec, Canada; ³Angiochem Inc., Montréal, QC, Canada; ⁴University of Montreal, Montreal, QC
- TP 330 **Studying the Sphingolipid Pathway into Co-morbidity of Depression and Alcoholism by MALDI Imaging FT-ICR Mass Spectrometry;** Christian P Muller¹; Matthias Witt²; Michael L Easterling³; Jens Fuchser²; Beckmann Janine²; Thomas Stockl¹; Eva Sprenger¹; Jens Tiesel¹; Sabine E Huber¹; Davide Amato¹; Erich Gulbins⁴; Martin Reichel¹; Johannes Kornhuber¹; ¹Department of Psychiatry and Psychotherapy, Friedrich-Alexander-University of Erlangen-Nuremberg, Erlangen, Germany; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics, Billerica, MA; ⁴Department of Molecular Biology, University of Duisburg-Essen, Essen, Germany
- TP 331 **Molecular Mapping of Gangliosides and Related Lipids using Mass Spectrometry Imaging with Ion Mobility Separation;** Bindesh Shrestha¹; Hernando Olivios²; Khaja Muneeruddin³; Miguel Sena-Estevés³; Scott A Shaffer³; ¹Waters Corp., Beverly, MA; ²Waters Corporation, Beverly, MA; ³University of Massachusetts Medical School, Worcester, MA
- TP 332 **Evaluating the Viability of Kidney Transplants using High-speed MALDI-Imaging;** Shane R Ellis¹; Tim C van Smaalen²; Nadine E Mascini^{1,3}; Berta Cillero-Pastor¹; Tiffany Porta¹; Benjamin Balluff¹; Carine J Peutz-Koostra²; L.W.E van Heurn⁴; Ron M A Heeren¹; ¹M4I, Maastricht University Maastricht, the Netherlands; ²Maastricht UMC+, Maastricht, Netherlands; ³FOM Institute AMOLF, Amsterdam, Netherlands; ⁴University of Amsterdam, Amsterdam, The Netherlands
- TP 333 **Proteomic Mass Imaging of Kidney from Type 2 Diabetes (T2D) Rat Model;** Hirata Chie¹; Kuzuhara Yuki¹; Iwasaki Noriyuki²; Kudo Toshiiji²; Nirasawa Takashi²; Masuyama Kei³; Kakuda Nobuto¹; Wakazono Hiroshi³; Yanagi Hiroyuki³; Masaya Ikegawa⁴; ¹Doshisha University, Kyotanabe, Japan; ²Bruker Daltonics K.K., Kanagawa, Japan; ³Ono Pharmaceutical Co., Ltd., Fukui, Japan; ⁴Doshisha University, Kyotanabe City
- TP 334 **Differentiating Macrophages in Atherosclerotic Plaques using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging;** Pegah Khamnehgir-Silz¹; Florian Schnitter²; Andreas H. Wagner²; Sabine Schulz¹; Markus Hecker²; Bernhard Spengler¹; ¹Justus Liebig University, Giessen, Germany; ²Ruprecht-Karls-University, Heidelberg, Germany
- TP 335 **What Can We Learn from the Na⁺/K⁺ Ratio in Imaging Mass Spectrometry Experiments?** Roberto Fernandez¹; Jone garate¹; Sergio Lage¹; Silvia Teres²; Pau Gonzalez³; Monica Higuera⁴; Alfredo Maqueda³; Joan Bestard-Escalas⁵; Daniel H Lopez⁵; Francisca Guardiola-serrano⁴; Pablo V Escibá⁴; Javier Rodriguez³; Gwendolyn Barceló-Coblijn⁵; Jose A. Fernandez⁶; ¹Universidad del Pais Vasco, Leioa,

Spain; ²Institut européen de chimie et biologie, Pessac, France; ³National Hospital for Paraplegics, Toledo, Spain; ⁴University of the Balearic Islands, Palma Balearic Islands, Spain; ⁵Institut d'Investigació Sanitària de Palma, Palma Balearic Islands, Spain; ⁶Universidad del País Vasco, leioa, Spain

TP 336 **Analysis of Retinal Degeneration in a Leber Congenital Amaurosis Mouse Model Using High Spatial Resolution MALDI-Imaging Mass Spectrometry;** David M. Anderson¹; Zsolt Ablonczy²; Yiannis Koutalos²; Nico Verbeeck³; Raf Van De Plas^{1,3}; Jeffrey Spraggins¹; Rosalie K. Crouch²; Richard M Caprioli¹; Kevin L. Schey¹; ¹Vanderbilt University MSRC, Nashville, TN; ²Department of Ophthalmology, Storm Eye Institute, Medical University of South, Charleston, SC; ³Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands

TP 337 **Molecular Target Validation in Human Atherosclerosis Based on Mass Spectrometry Imaging and ImmunHistoChemistry Evaluation;** Jonathan Stauber¹; Gregory Hamm¹; Sylvia Aldi²; Juliette Masure¹; Kim Holmstrom³; Serife Arda⁴; Danielle Van Keulen^{5,6}; David Bonnel¹; Ivana Bobeldijk-Pastorova⁵; Dennie Tempel⁶; Boye S Nielsen³; Michael Gudo⁴; Jan NH Lindeman⁷; Ulf Hedin²; Alain van Gool⁵; Eva Hurt Camejo⁸; ¹ImaBiotech, MS Imaging Dept. Loos, France; ²Department of Molecular Medicine and Surgery, Karolinska Institutet, Stockholm, Sweden; ³Bioneer, Hoersholm, Denmark; ⁴Morphisto, Frankfurt Am Main, Germany; ⁵TNO, Metabolic Health Research Leiden, The Netherlands; ⁶CardioGenx, Rotterdam, The Netherlands; ⁷Leiden University Medical Centre, Leiden, The Netherlands; ⁸AstraZeneca R&D, Gothenburg, Sweden

TP 338 **Simultaneous Detection of N-glycans and Peptides from a Single FFPE Tissue Section by MALDI FT-ICR Imaging Mass Spectrometry;** Peggy Angel¹; Rita Casadonte²; Jörg Kriegsmann²; Richard Drake³; ¹Medical University of South Carolina, Charleston, SC; ²Proteopath GmbH, Trier, Germany; ³Medical Univ of S Carolina, Charleston, SC

TP 339 **The Effect of Oxygen on the Lipid Composition of Human Chondrocytes using MALDI Imaging;** Brenda Bakker¹; Gert Eijkel²; Ron Heeren²; Marcel Karperien¹; Janine Post¹; Berta Cillero-Pastor²; ¹Developmental BioEngineering, University of Twente, Enschede, The Netherlands; ²The Maastricht Multimodal Molecular Imaging Institute (M4I), Maastricht University, Maastricht, The Netherlands

TP 340 **Metabolite Profiling of Intestinal Microbiota by Mass Spectrometry Imaging for Biological Understanding of Gastrointestinal Disease;** Gregory Hamm¹; Juliette Masure¹; Sylvain Normand²; David Bonnel¹; Mathias Chamaillard²; Jonathan Stauber¹; ¹ImaBiotech, MS Imaging Dept. Loos, France; ²Center of Infection and Immunity of Lille (CIIL), Team 7, Inserm U1019, CNRS UMR8204, Lille, France

TP 341 **Differential Human Pancreatic Lipid and Protein Distributions in Normal and Type 1 Diabetes Revealed by Tissue Imaging Mass Spectrometry;** Boone M. Prentice¹; Rachana Haliyur¹; Nathaniel J Hart¹; Audra M Judd¹; Radhika Aramanda¹; Marcela Brissova¹; Jeffrey M Spraggins¹; Jeremy L Norris¹; Alvin C Powers¹; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN

TP 342 **Lipid and Metabolite Distribution in Healthy and Diseased Brain Tissue using DESI and High Resolution Mass Spectrometry;** Joseph H Kennedy¹; Jeff Patrick¹; Mariam ElNaggar¹; Justin M Wiseman¹; ¹Prosolia, Inc. Indianapolis, IN

TP 343 **Imaging Mass Spectrometry for the Pathological Studies of Cardiac Allografts;** Terada Megumi¹; Iwasaki Noriyuki²; Kudo Toshiiji²; Nirasawa Takashi²; Bruneval

Prtrick³; Ishibashi-Ueda Hatsue⁴; Masaya Ikegawa⁵; ¹Doshisha University, Graduate School of Brain Scie Kyoto, Japan; ²Bruker Daltonics K.K., Kanagawa, Japan; ³Georges Pompidou European Hospital, Paris, France; ⁴National Cerebral and Cardiovascular Center, Osaka, Japan; ⁵Doshisha University, Kyotanabe City

TP 344 **High Spatial Resolution Lipid Imaging Offers Promising Perspectives in Sustaining Diagnosis of Human Lymphoma;** Yousef El Aalamat¹; Arndt Asperger²; Xian Mao¹; Wim Waelput³; Thomas Tousseyn⁴; Bart De Moor¹; Etienne Waelkens⁵; ¹ESAT-STADIUS / iMinds Medical IT, KU Leuven, Leuven, Belgium; ²shared first author, Bruker Daltonik GmbH, Bremen, Germany; ³Dept. of Pathology, UZ-Brussel, Brussel, Belgium; ⁴Dept. Imaging and Pathology, KU Leuven, Leuven, Belgium; ⁵Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium

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TP 345 **Towards Absolute Quantitative MALDI MS Imaging of Drugs;** Patrik Kallback¹; Theodosia Vallianatou²; Anna Nilsson²; Mohammadreza Shariatgorji²; Per E Andren²; ¹Uppsala University, Uppsala, Uppsala; ²Uppsala University, Uppsala, Sweden

TP 346 **Derivatization Strategies for the Quantitation of Triamcinolone Acetonide in Cartilage by using Imaging Mass Spectrometry;** Florian Barré¹; Bryn Flinders¹; Joao Garcia²; Laura Creemers²; Ron M A Heeren¹; Berta Cillero-Pastor¹; ¹M4I Institute - Maastricht University, Maastricht, The Netherlands; ²Utrecht University, Utrecht, The Netherlands

TP 347 **3D MALDI Mass Spectrometry Imaging to Empower Drug Distribution And Quantitation Studies in Solid Tumors;** Silvia Giordano¹; Lavinia Morosi¹; Pietro Veglianesi¹; Simonetta Andrea Licandro¹; Roberta Frapolli¹; Massimo Zucchetti¹; Maurizio D'Incalci¹; Enrico Davoli¹; ¹IRCCS Istituto Mario Negri, Milano, Italy

TP 348 **Study of the Blood Brain Barrier Permeability using a Multimodal Imaging Approach;** David Calligaris¹; Fa-Ke Lu¹; Armen Changelian¹; Isaiah Norton¹; Brett L Carlson²; Jeffrey Agar³; William F Elmquist⁴; Daniel MA²; Jann N Sarkaria²; Nathalie YR Agar¹; ¹Department of Neurosurgery, Brigham and Women's Hospital - Harvard Medical School, Boston, MA; ²Mayo Clinic, Rochester, MN; ³Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA; ⁴Department of Pharmaceuticals, University of Minnesota, Minneapolis, MN

TP 349 **Comparison of LESA-MS to MALDI-MS for Mouse Whole Body Tissue Profiling: Diclofenac and Major Metabolites;** Walter Korfmacher¹; Gargey Yagnik²; Yongyi Luo³; Stacy Ho²; Liduo Shen³; Terry Wilper⁴; Karen Norton⁴; Eric Solon⁵; Hanlan Liu²; Sara Savage⁴; Thomas O'Shea²; ¹Genzyme, Waltham, MA; ²Genzyme, a Sanofi company Waltham, MA; ³Sanofi, Waltham, MA; ⁴Genzyme, Framingham, MA; ⁵QPS, Newark, DE

TP 350 **Matrix Assisted Laser Desorption/Ionisation Mass Spectrometry Imaging of Therapeutic Oligonucleotides: Application to Antisense Therapy;** C. Logan Mackay¹; John G Swales²; Richard J A Goodwin²; ¹SIRCAMS, Edinburgh, UK; ²AstraZeneca, Cambridge, UK

TP 351 **Microinjection and High-throughput Alignment of Cellular Spheroids for MALDI Mass Spectrometry Imaging Analysis;** Jillian Johnson¹; Fengfei Ma¹; Weiyuan John Kao¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

TP 352 **Applications of Single-Probe Device for Ambient Mass Spectrometry Imaging Analysis: Human Corneas and 3D Artificial Tumors;** Xiang Tian¹; Wei Rao¹; Ning Pan¹; Haiqing Yu¹; Dimitrios Karamichos²; Zhibo Yang¹; ¹University

- of Oklahoma, Dept. of Chem & Biochem Norman, OK; ²University of Oklahoma Health Science Center, OKC, OK
- TP 353 **Application of Imaging Mass Spectrometry to Assess Ocular Drug Transit**; Kerri Grove¹; Viral Kansara²; Melissa Prentiss²; Debby Long²; Muneto Mogi²; Sean Kim²; Patrick Rudewicz¹; ¹Novartis Institutes for BioMedical Research, Emeryville, CA; ²Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA
- TP 354 **MALDI-FTICR Imaging of the Distribution of Teriflunomide in CNS Tissues in an Experimental Model of Multiple Sclerosis**; Ignacy Rzagalinski¹; Carola Meier¹; Nadine Hainz¹; Thomas Tschernig¹; Dietrich Volmer¹; ¹Saarland University, Saarbrücken, Germany
- TP 355 **Multimodal Mass Spectrometry Imaging for Detection and Early Prediction of Drug Induced Phospholipidosis**; Richard Goodwin¹; Anna Nilsson²; Jennifer Barnes¹; Julia Sampson¹; Hui Zhang³; John G Swales¹; Nicole strittmatter⁴; Alan Race⁵; Rory Steven⁶; Logan C Mackay⁶; Josephine Bunch⁶; Per E Andren²; ¹AstraZeneca, Cambridge, UK; ²Uppsala University, Uppsala, Sweden; ³AstraZeneca R&D, Mölndal, Sweden; ⁴AstraZeneca, Macclesfield, Select State; ⁵National Physical Laboratory, Teddington, United Kingdom; ⁶University of Edinburgh, Edinburgh, United Kingdom
- TP 356 **The Evaluation of Erythroblast Dynamics in Mice Bone Marrows by MALDI FTICR-MS Imaging which Identifies 57Fe-labeled Heme Isotopic Fine Structure**; Makoto Kihara¹; Yukari Matsuo-Tezuka²; Keigo Yorozu²; Mitsue Kurasawa²; Hideyuki Yasuno²; Yasushi Shimomaka²; ¹Chugai Pharmaceutical Co., Ltd, Kamakura, Japan; ²Chugai Pharmaceutical Co., Ltd Kamakura, Japan
- TP 357 **Large Scale, Multi-Instrument MALDI-MSI Study into Lipidosis in Inhalation Dosed Rats**; Rory Thomas Steven¹; Alan Race¹; Aateka Patel²; Lea Ann Dailey²; Josephine Bunch^{1,3}; ¹National Physical Laboratory, Teddington, UK; ²King's College London, London, UK; ³University of Nottingham, Nottingham, UK
- TP 358 **MALDI Imaging Mass Spectrometry of Platinum-Based Drugs in Multicellular Tumor Spheroids (MCTS) using Derivatization with Diethyldithiocarbamate (DDTC)**; Xin Liu¹; Amanda B Hummon¹; ¹University of Notre Dame, Notre Dame, Indiana
- TP 359 **Visualization of Small Molecule and Nanoparticle Anticancer Agents in Tissue and Tumor Sections using IR-MALDESI Mass Spectrometry Imaging**; Mark Bokhart¹; Allison Schorzman²; Andrew Lucas²; Michael Berens³; Harshil Dhruv³; William Zamboni²; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²UNC - Chapel Hill, Chapel Hill, NC; ³Translational Genomics Research Institute, Phoenix, AZ
- TP 360 **Tissue Distribution of Compound X and its Metabolites in Jck Mouse Polycystic Kidneys using Mass Spectrometry Imaging (MSI)**; Hanlan Liu¹; Cristina Silvescu¹; Mandy Cromwell²; Kelly Keefe²; Lindsay Quigley²; Sirimas Sudsakorn¹; Sarah Nsereko¹; Yang Guo¹; Laurie Smith³; Thomas Natoli³; Dinesh Bangari⁴; Gregory Hamm⁵; Aurore Tomezyk⁶; Raphael Legouffe⁶; David Bonnel⁶; Jonathan Stauberand⁶; Thomas O'Shea¹; ¹Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; ²Rare Disease Pharmacology, Sanofi, Waltham, MA; ³Rare Renal Disease Research, Sanofi, Framingham, MA; ⁴Pathology, Sanofi, Framingham, MA; ⁵ImaBiotech, MS Imaging Dept. Loos, France
- TP 361 **Visualizing Anti-Retroviral Distribution in Sheep and Human Vaginal Tissue by Imaging Mass Spectrometry**; Michelle Reyzer¹; Mark Marzinko²; Trevelyn Olive³; Richard Pyles³; Kathleen L Vincent³; Manjula Gunawardana⁴; John Moss⁴; Marc M. Baum⁴; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²Johns Hopkins University, Baltimore, MD; ³University of Texas Medical Branch at Galveston, Galveston, TX; ⁴Oak Crest Institute of Science, Monrovia, CA
- TP 362 **MALDI IMS in Drug Development: Shedding New Light on Toxicology**; M. Reid Groseclose¹; Stephen Castellino¹; ¹GlaxoSmithKline, Upper Merion, PA
- TP 363 **Complementary Elemental And Molecular Mass Spectrometry Imaging to Investigate 5-aminolevulinic Acid, Protoporphyrin IX and Heme Distribution in Human Brain Tumor**; Sabrina Kröger¹; Ann-Christin Niehoff¹; Uwe Karst¹; ¹University of Münster, Institute of Inorganic and Analytical Chemistry, Münster

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- TP 364 **Resolving Complex Glycopeptide Fragmentation Tandem Mass Spectrum**; Aiyang Yu¹; Lauren Zacharias¹; Rui Zhu¹; Kerry Wooding¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
- TP 365 **Recycling Modification Site Information for Improved Glycopeptide Analysis**; Robert Chalkley¹; Peter R Baker¹; ¹UCSF, San Francisco, CA
- TP 366 **Decoding Histone Post-translational Modifications by Bottom-up Mass Spectrometry**; Zuo-Fei Yuan¹; Simone Sidoli¹; Shu Lin¹; Xiaoshi Wang¹; Natarajan V Bhanu¹; Benjamin A Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- TP 367 **Peak Annotation of High Resolution Spectra for Constructing Peptide Mass Spectral Libraries**; Xiaoyu Yang¹; Pedatsur Neta¹; Yuri Mirokhin¹; Dmitrii Tchekhovskoi¹; Yuxue Liang¹; Zheng Zhang¹; Sergey Sheetlin¹; Sanford Markey¹; Stephen Stein¹; ¹NIST, Gaithersburg MD
- TP 368 **A New Hope for Label Free Proteomics: moFF for Open-source, Platform-independent, Automated MS1 Intensity Extraction**; andrea argentine^{1,2,3}; Kenneth Verheggen^{1,2,3}; Lennart Martens^{1,2,3}; ¹Medical Biotechnology Center, VIB, Gent, Belgium; ²Department of Biochemistry, Ghent University, Ghent, Belgium; ³Bioinformatics Institute Ghent, Ghent University, Ghent, Belgium
- TP 369 **Interconversion of Peptide Spectral Libraries between iTRAQ and TMT Labels**; Zheng Zhang¹; Xiaoyu Yang¹; Yuri A Mirokhin¹; Dmitrii V Tchekhovskoi¹; Weihua Ji¹; Sanford P Markey¹; Jeri Roth¹; Deniz BaycinHizal²; Michael Bowen²; Stephen E Stein¹; ¹NIST, Rockville, MD; ²MedImmune, Gaithersburg, MD
- TP 370 **Employing Complementary Ions for Deconvolution of Mixture Tandem Mass Spectra**; Vladimir Gorshkov¹; Stéphanie Yuki Kolbeck Hotta¹; Thiago Verano-Braga^{1,2}; Frank Kjeldsen¹; ¹University of Southern Denmark, Odense, Denmark; ²Federal University of Minas Gerais, Belo Horizonte, Brazil
- TP 371 **Combination of MS3/HCD and MS2/CID Improves Peptide IDs in Addition to Reducing the Precursor Interference of TMT-quantitation Experiment**; Wen Yu¹; Raghothama Chaerkady¹; Deniz Baycin-Hizal¹; Mathew Woodward²; Michael A Bowen¹; ¹MedImmune, Gaithersburg, MD - Maryland; ²MedImmune, Cambridge, UK
- TP 372 **The Benefits of Recycling – Protein Prospector: the Eco-Friendly Search Engine**; Peter R Baker¹; Juan A Osés²; Robert J Chalkley²; ¹UCSF, Rokitnica; ²UCSF, San Francisco, CA
- TP 373 **Evaluating Software for Precursor Ion Chromatograms in Label-Free Data-Dependent Acquisition Sets through Differentiation, Quantification, and Clustering**; Yasset Perez-Riverol¹; Chao Liu²; Bridget Calder³; Suereta Fortuin³; Alexander Giddey³; Birgit Schilling⁴; David Lee Tabb⁵; ¹EMBL-EBI, Hinxton, UK; ²Institute of Computing Technology, CAS Beijing, CHINA; ³University of Cape Town, Cape Town, ZA; ⁴Buck Institute for Research on Aging, Novato, CA; ⁵Stellenbosch University, Liberty, MO

- TP 374 **Identification of Host Cell Protein Impurities using Spectral Libraries;** Meghan Burke¹; Yuxue Liang¹; Kelly H. Telu¹; Jenny Heidbrink Thompson²; Chris Larkin²; Stephen Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²MedImmune, Gaithersburg, MD
- TP 375 **Negative Electron Transfer Dissociation Fragmentation in a Full-Featured Proteomics Search Engine;** Yong J. Kil¹; Wilfred Tang²; Nicholas M Riley³; Michael S Westphall³; Joshua J Coon³; Marshall W. Bern²; ¹Protein Metrics, San Carlos, CA; ²Protein Metrics, Palo Alto, CA; ³University of Wisconsin Madison, Madison, Wisconsin
- TP 376 **Fast and Comprehensive Peptide Identifications through Index-based Database Search;** Andy Kong¹; Felipe de Veiga Leprevost¹; Alexey I Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- TP 377 **A Graph-Centric Approach for Metagenome-Guided Peptide Identification in Metaproteomics;** Sujun Li¹; Yuzhen Ye¹; Haixu Tang¹; ¹Indiana University, Bloomington, IN
- TP 378 **Large Scale Silac Based Quantitative Analysis of Electron Acceptor Stressed Azospira Suillum PS using Retention and Drift Time Profiling;** Anthony T Iavarone¹; Matthew D Youngblut¹; Emilie Gios¹; Michael Daly²; Hans K Carlson¹; Ulla N Andersen¹; Johannes PC Vissers³; John D Coates¹; ¹UC Berkeley, Berkeley, California; ²Waters, Inc. Pleasanton, CA; ³Waters, Wilmslow, United Kingdom
- TP 379 **PGA: an R Package for Identification of Novel Peptides by Customized Database Derived from RNA-Seq;** Bo Wen¹; Shaohang Xu¹; Ruo Zhou¹; Bing Zhang²; Wang Xiaojing²; Xin Liu¹; Xun Xu¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China; ²Vanderbilt University School of Medicine, Nashville, TN
- TP 380 **The Systemic MHC Atlas Project: toward a First Mass Spectrometry-based Draft of the Human Immunopeptidome;** Witold Wolski¹; Etienne Caron²; Heiko Schuster; Michal Bassani-Sternberg³; Lorenz Blum⁴; Christian Panse⁵; Ruedi Aebersold²; Ralph Schlapbach⁵; ¹FGCZ ETH Zurich, Zurich, Not US or Canada; ²Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; ³UNIL/CHUV Ludwig Cancer Research Center Lausanne, Switzerland, Lausanne, Switzerland; ⁴ETH Zurich, Zurich, Switzerland; ⁵FGCZ, Univ Zurich Zurich, Switzerland
- TP 381 **An Approach to Explore Millions of Unidentified MS/MS Peptide Features with Network Modeling and Its Implication for In-depth Proteomics;** Paul E Abraham¹; John C Cushman²; Daniel Jacobson¹; Robert L Hettich¹; Richard J Giannone¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Nevada, Reno, Reno, NV
- TP 382 **Should We Care about Peptide Co-elution?** ; Jamie Sherman¹; Stephen Tate¹; ¹SCIEX, Concord ON, Canada
- TP 383 **Solving the "no-enzyme" Problem in MHC-peptide immuno-precipitation Database Searches;** Patrick Murphy¹; Konda Prathyusha¹; Clements Derek¹; Heiko Schuster²; Daniel Kowalewski²; Brian Erickson³; Joao Paulo³; Alejandro Cohen⁴; Steven P Gygi³; Stefan Stevanovic²; Shashi Gujar¹; Patrick Lee¹; ¹Dalhousie University Dept of Microbiology and Immunology, Halifax, Canada; ²University of Tuebingen, Tuebingen, Germany; ³Harvard Medical School, Boston, MA; ⁴Dalhousie University, Department of Chemistry Halifax, Canada
- TP 384 **New Calibration and Absolute Quantification Features in Skyline;** Nicholas Shulman¹; Clark Henderson¹; Birgit Schilling²; Will J Thompson³; Christopher M Shuford⁴; Andy Hoofnagle¹; Michael J MacCoss¹; Brendan MacLean¹; ¹University of Washington, Seattle, WA; ²Buck Institute for Research on Aging, Novato, CA; ³Duke University, Durham, NC; ⁴Center for Esoteric Testing, Burlington, NC
- TP 385 **De novo Sequencing of Peptides from High-resolution Bottom-up Tandem Mass Spectra using Top-down Intended Methods;** Kira Vyatkina^{1,2}; Lennard J.M. Dekker³; Si Wu⁴; Martijn M. Vanduijn³; Xiaowen Liu^{5,6}; Nikola Tolic⁷; Theo M. Luider³; Ljiljana Pasa-Tolic⁷; Pavel A. Pevzner⁸; ¹Saint Petersburg State University, St Petersburg, Russian Federation; ²Saint Petersburg Academic University, St Petersburg, Russia; ³Erasmus Medical Center, Rotterdam, The Netherlands; ⁴University of Oklahoma, Dept. of Chem & Biochem Norman, OK; ⁵Indiana University-Purdue University Indianapolis, Indianapolis, IN; ⁶Indiana University School of Medicine, Indianapolis, IN; ⁷Pacific Northwest National Laboratory - PNNL, Richland, WA; ⁸University of California, San Diego La Jolla, CA
- TP 386 **Advanced XIC-based Label-free Algorithm for High-Resolution Data;** Sung Kyu Robin Park¹; Rohan Rampuria²; Khatereh Motamedchaboki³; Jolene Diedrich²; Claire Delahunty²; John R Yates²; ¹The Scripps Research Institute, San Diego, CA; ²The Scripps Research Institute, La Jolla, CA; ³Sanford-Burnham Medical Research Institute, La Jolla, CA
- TP 387 **Pros and Cons of Large Scale MS/MS Clustering - Are We There Yet?;** Benjamin Pullman^{1,2}; Nuno Bandeira^{1,2,3}; ¹Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; ²Computer Science and Engineering, University of California San Diego, La Jolla, CA; ³Skaggs School of Pharmacy, UC San Diego La Jolla, CA
- TP 388 **Combining RNA-Seq Proteogenomics and Global Post-Translational Modification (G-PTM) Search Strategy to Reveal Human Proteomic Variation;** Anthony J Cesnik¹; Michael R Shortreed¹; Gloria M Sheynkman¹; Brian L Frey¹; Lloyd M Smith¹; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- TP 389 **A New Database Format to More Closely Examine Protein Splice Forms;** Aparna Nathan¹; Waltraud Mair¹; Jan Muntel¹; Hendrik Wesseling¹; Judith Steen¹; Hanno Steen¹; ¹Boston Children's Hospital, Boston, MA
- TP 390 **Challenges and Solutions When using OpenMS LFPProfiler Node in Proteome Discoverer 2.1 for Feature Comparison in Very Large Datasets;** Jana Moerbe Rucker¹; Lindsay Schambeau¹; Lewis K Pannell¹; ¹University of South Alabama, Mobile, AL
- TP 391 **New Method for Label-free Quantification in the Proteome Discoverer Framework;** David Horn¹; Torsten Ueckert²; Kai Fritzemeier²; Carmen Paschke²; Katja Tham²; Hans Pfaff²; Xiaoyue Jiang³; Joseph Brown³; Iman Mohtashemi¹; Daniel Lopez Ferrer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, DE; ³Thermo Fisher Scientific, San Jose, CA

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- TP 392 **Control Software for a Spatially Multiplexed Ion Mobility-Mass Spectrometer;** Babatunde H. Bello^{1,2}; Katrina L. Leaptrout^{2,3}; Jody C. May²; John A. McLean^{2,3}; ¹Department of Mechanical Engineering, Vanderbilt University, Nashville, TN; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³VIBRE, Vanderbilt University, Nashville, TN
- TP 393 **Real-Time Instrument Control of the Orbitrap Tribrid Mass Spectrometer;** Derek J Bailey¹; Florian Grosse-Coosmann²; Manish Doshi¹; Qingyu Song¹; Jesse D Canterbury¹; Qiming Wan¹; Michael Senko¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, DE
- TP 394 **High-Sensitive MCP-based Ion Detector for Time of Flight Mass Spectrometry using Triode Structure;** Masahiro Hayashi¹; Tetsuya Matsushita¹; Joji Sakakiyama¹; Akio Suzuki¹; Toshiyuki Uchiyama¹; Yasuhide Naito²;



- ¹Hamamatsu Photonics K.K., Iwata, Japan; ²GPI, Hamamatsu, Japan
- TP 395 **Improved Detection Efficiency of a High Dynamic Range Pulse Counting Detection System;** Bruce Collings¹; Martine Dima¹; Pascal Martin¹; Stephen Bruce Locke¹; ¹SCIEX, Concord, ON
- TP 396 **Highly Charge-sensitive Device to Enhance the Direct Detection of Molecular Ions;** Szu-Wei Chou¹; Yao-Hsin Tseng¹; Liang-Chun Fan¹; Yi-Kun Lee¹; Chun-Yen Cheng¹; ¹AcroMass Technologies, Inc. Taipei, Taiwan
- TP 397 **A New Method for Measuring Detector Operating Life Performance;** Toby Shanley¹; Clifton Chey¹; Russell Jurek¹; Kevin L Hunter¹; Peter Raffin¹; Daen Ekers¹; Wayne Sheils¹; ¹ETP Ion Detect, Clyde, Australia
- TP 398 **A Method for Controlling Collective Electron Motion in Ion Detectors by Locally Manipulating Magnetic Fields;** Toby Shanley¹; Russell Jurek¹; Yair Benari¹; Dick Stresau¹; Kevin L Hunter¹; ¹ETP Electron Multipliers, Clyde, Australia
- TP 399 **Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection;** Lisa Cousins¹; Heather Gamble¹; Charles Joliffe¹; Joshua Ye¹; Jason Courmoyer²; ¹Ionics, Bolton, Canada; ²PerkinElmer, Waltham, MA
- TP 400 **Evaluation of RF-phase during Photoionization on the Trapping and Ejection of Ions from a 3D Ion Trap;** Laura Bailey¹; Matthew R. Bell¹; Nicolas C Polfer¹; ¹University of Florida, Gainesville, FL
- TP 401 **Implementation of Ultraviolet Photodissociation using Light Emitting Diodes (LEDs) in an Ion Trap;** Dustin D. Holden¹; Alexander Makarov²; Jae C Schwartz³; James D Sanders¹; Eugene Zhuk³; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Thermo Fisher Scientific, Bremen, DE; ³Thermo Fisher Scientific, San Jose, CA
- TP 402 **Improving the Performance of a Wysocki SID Cell for Synapt HDMS;** Mehdi Shirzadeh¹; David H Russell¹; ¹Texas A&M, College Station, TX
- TP 403 **ECD Analysis of Serine Phosphorylated Peptides using EMS Cell;** Valery G. Voinov¹; Yury V Vasil'ev¹; Douglas F Barofsky²; Joseph Beckman¹; ¹Linus Pauling Institute, Oregon State University Corvallis, OR; ²Oregon State University, Department of Chemistry Corvallis, OR
- TP 404 **Up Front CID in a Laminar Flow Ion Guide for Performance Enhancement in Biological Samples;** Charles Joliffe¹; Shah Joshua Ye¹; Heather Gamble¹; Devanand Pinto²; Andrew Leslie²; ¹Ionics, Bolton, Canada; ²National Research Council of Canada, Halifax, Canada
- TP 405 **Design and Modeling of a Long Distance Low Vacuum Ion Transfer System;** Roman Levin^{1,2}; Evgeny Zhvansky^{1,2}; Vasily Eliferov^{1,3}; Igor Popov^{1,2}; Alexey Boldyrev²; Gleb Vladimirov²; Eugene Nikolaev²; ¹Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation
- TP 406 **Efficient Ion Transmission and Desolvation Enabled by Vortical Flow in DRy Ion Localization and Locomotion (DRILL) MS interface;** Jung Lee¹; Peter Kottke¹; Elizabeth S Hecht²; David C Muddiman²; Nagender Panyala¹; Matthew Torres¹; Andrei Fedorov¹; ¹Georgia Institute of Technology, Atlanta, GA; ²NC State University, Raleigh, NC
- TP 407 **A Mass Selective Transfer Line for Injecting Ions in a Uniform Supersonic Flow;** Baptiste Joalland¹; Ludovic Biennier¹; Sophie Carles¹; Alexander Lekkas²; Dimitris Papanastasiou²; Emmanuel Raptakis²; ¹Institut de Physique de Rennes, CNRS - Université de Rennes 1, Rennes, FR; ²Fasmatech, Athens, Greece
- TP 408 **Ion Transport through Zirconia Capillaries;** J. A. Jarrell; Waters Corporation, Milford, MA
- TP 409 **Development of Ultra-High Resolution Biological Target Characterization Mass Spectrometry Instrumentation;** Raul Villacob¹; Paolo Benigni¹; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL
- TP 410 **Coupling Raman Spectroscopy with Laser Desorption-Atmospheric Pressure Chemical Ionization/Mass Spectrometry (LD-APCI/MS) for Polymer Analysis;** Yen-Ting Chen¹; Siou-Sian Jhang¹; Jentaie Shiea¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan
- TP 411 **Thermogravimetric Analyzer Coupled with Atmospheric Pressure Chemical Ionization/Mass Spectrometry (TGA-APCI/MS) to Characterize Polymers in Biodegradable Plastics Materials;** Yao Sheng Zhang¹; Sheng Hui Chiu¹; Ming Chen¹; Siou Sian Jhang¹; Jentaie Shiea¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan
- TP 412 **Fully Automated Analysis Platform for the Routine Determination of Immunosuppressants in Whole Blood;** Daide Vecchiotti¹; Maura Brambilla²; Daisuke Kawakami³; Taku Tsukamoto³; Paolo Brambilla²; ¹Shimadzu, Milan, Lombardy; ²Desio Hospital, Toxicology and Mass spectrometry department, Desio, Italy; ³Shimadzu Corporation, Kyoto, Japan
- TP 413 **Automated Bottom-up Proteomics Workflow for Liquid AP-MALDI MS/MS Utilising Multiply Charged Ions;** Pavel Ryumin¹; Jeff Brown^{1,2}; Michael Morris²; Rainer Cramer¹; ¹University of Reading, Reading, United Kingdom; ²Waters, Wilmslow, United Kingdom
- TP 414 **A New Conjoined RF Ion Guide for High Efficiency Ion Transmission;** Daniel Kenny¹; David Gordon¹; Kevin Giles¹; ¹Waters, Wilmslow, United Kingdom
- TP 415 **Performance Monitoring and Quadrupole Maintenance of a First Generation Q Exactive Orbitrap in a Core Facility Setting;** John Leszyk¹; Scott A Shaffer¹; ¹UMass Medical School, Shrewsbury, MA
- TP 416 **Building a Next-Generation Platform for Electron-ion Optics Simulations;** Russell Jurek^{1,2}; Kevin L Hunter³; ¹ETP Ion Detect, Clyde, Australia; ²ETP Ion Detect, Clyde, Australia; ³ETP Ion Detect, Clyde, Australia

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- TP 417 **Development and Characterization of an FT-QIT with in situ Electron Ionization for Residual and Trace Gas Analysis;** Yessica Brachthaeuser¹; David Mueller¹; Hendrik Kersten¹; Klaus Brockmann¹; Thorsten Benter¹; Valerie Derpmann²; Alexander Laue²; Ruediger Reuter²; Michel Aliman²; ¹Bergische Universität Wuppertal, Wuppertal, Germany; ²Carl Zeiss SMT GmbH, Oberkochen, Germany
- TP 418 **Study of Directional Ion Ejection in an Asymmetric Half-Round Rod Electrode Linear Ion Trap Mass Analyzer;** Zhang Zaiyue¹; Yuan Guangzhou¹; Qian Jie¹; He Yang¹; Yao Rujiao¹; Zhang Shuguang¹; Xiaoxu Li¹; ¹Soochow University, Suzhou, China
- TP 419 **Optimization of the Mesh-electrode Linear Ion Trap Performance by Simulations;** Qiankun Dang¹; Gary Glish²; Chuan-Fan Ding³; ¹Fudan University, Shanghai, Shanghai; ²University of North Carolina at Chapel Hill, Chapel Hill, NC; ³Fudan University, Shanghai, China
- TP 420 **Improvement of Mass Resolution, Collision Induced Dissociation Efficiency and Low Mass Cutoff by Octopole Field in Linear Ion Trap Mass Analyzer;** Chuan-Fan Ding¹; Fuxing Xu²; Xinhua Dai³; Xiang Fang³; ¹Fudan University, Shanghai; ²Fudan University, Shanghai, China; ³National Institute of Metrology, Beijing, China
- TP 421 **Design and Analytical Performance Evaluation of a Cooling Cell for a Quadrupole Mass Spectrometer with Enhanced Resolution and Sensitivity;** Tsung-Chi Chen¹; Philip M Remes¹; Raman Mathur¹; Paul H Gregory¹;



- Pascual Cardenas¹; Rexford T Heller¹; Qingyu Song¹; Viatcheslav V Kovtoun¹; Satendra Prasad¹; Hoa D Truong¹; Eloy R Wouters¹; Hans Schweingruber¹; Eric C Hemenway¹; Jae C Schwartz¹; Terry N Olney¹; Alan E Schoen¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 422 **Effects of Hexapole Electric Fields on the Performance of Linear Ion Trap Mass Analyzer;** Fuxing Xu¹; Xinhua Dai²; Xiang Fang²; Yuanyuan Wang¹; Chuan-fan Ding¹; ¹Fudan University, Shanghai, China; ²National Institute of Metrology, Beijing, China
- TP 423 **Reducing Space Charge Effects in a Linear Ion Trap by Rhombic Ion Excitation and Ejection;** Lili Hu¹; Xiaohua Zhang²; Yuzhuo Wang³; Dan Guo¹; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, China; ²Fudan University, Shanghai, China; ³National Institute of Metrology, Beijing, China
- TP 424 **Ion Collision Cross Section Analyses in Quadrupole Ion Traps using Filter Diagonalization Method:** A Theoretical Study; Ting Jiang¹; He Mui¹; Guo Dan¹; Zhai Yanbing¹; Xu Wei¹; ¹Beijing Institute of Technology, Beijing, China
- TP 425 **Ion Trap Fourier Transform Mass Spectrometer with Induced Current Detection and Arbitrary Storage Waveforms;** Michael W Schmidt¹; Albrecht Brockhaus¹; Stefan Butzmann¹; Michel Aliman²; Alexander Laue²; ¹University of Wuppertal, Wuppertal, Germany; ²Carl Zeiss SMT GmbH, Oberkochen, Germany
- TP 426 **Improved Performance of Ion Trap Mass Spectrometer with Added Octopole and Dodecapole Fields;** Junichi Taniguchi; Shimadzu Corp., Soraku-gun, Kyoto
- TP 427 **Demonstration of using Isolation Waveform for Beam Type Selected-Reaction-Monitoring on a QqLIT Mass Spectrometer;** Qingyu Song¹; Jae C Schwartz¹; Philip M Remes¹; Dumitrescu Dean¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 428 **Advancements in Multi Reflecting High Resolution TOF Mass Spectrometry with Folded Flight Path;** Viatcheslav Artaev¹; Michael Mason¹; Peter A Willis¹; George Tikhonov¹; Yury Khasin²; Anatoly Verenchikov²; ¹LECO Corporation, St Joseph, MI; ²MSC-CG, Bar, Montenegro
- TP 429 **A Study of Ion Acceleration in tightly Curved Collision Cells;** Felician Muntean¹; Desmond A Kaplan¹; ¹Bruker Daltonics, Inc., Billerica, MA
- TP 430 **Performance of the Orbitrap Fusion Lumos Tribrid in Single-shot Analyses of Human Samples;** Guadalupe Espadas^{1,2}; Eva Borràs^{1,2}; Cristina Chiva^{1,2}; Eduard Sabidó^{1,2}; ¹Proteomics Unit, Center for Genomic Regulation, Barcelona, Spain; ²Proteomics Unit, Universitat Pompeu Fabra, Barcelona, Spain
- TP 431 **NTOF Geometry for QqTOF;** Bill Loyd¹; Robert E. Haufler²; ¹SCIEX, Concord, ON; ²AB Sciex, Concord, ON
- TP 432 **Optimization of the Performance of Toroidal Ion Trap by Theoretical Simulation;** Haiyang yang¹; Chengsheng Xu²; Chuan-Fan Ding²; ¹Fudan University, Shanghai; ²Fudan University, Shanghai, China
- TP 433 **A Mathematical and Simulation Study of General Toroidal Ion Trap Mass Spectrometer Devices;** Robert H Jackson¹; Steve Lammert²; Daniel Austin³; Karl Warnick³; Jessica Higgs³; Edgar Lee²; ¹Instrumental Design Physics, LLC, Littleton, MA; ²PerkinElmer, Inc., American Fork, UT; ³Brigham Young University, Provo, UT
- TP 434 **Radio Frequency Trapping of Ions in a Pure Toroidal Potential Distribution;** Jessica Higgs¹; Brae V. Petersen¹; Steven A. Lammert²; Karl F. Warnick¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT; ²PerkinElmer, American Fork, UT
- TP 435 **Simulation of Ion Motion in Non-Ideal Electric Fields Generated by Novel FTICR Mass Analyzers;** Joshua Driver¹; Andriy Kharchenko¹; Jon Amster¹; ¹Univ of Georgia, Athens, GA
- TP 436 **Cross-field Drift of Ions and Non-Linear ICR Cell Arrays;** Sung-Gun Park¹; Gordon Anderson²; James Bruce¹; ¹University of Washington, Seattle, WA; ²GAA Custom Engineering, LLC, Benton, WA
- TP 437 **Moving Practical Mass Spectrometry Beyond the Molecular Realm;** Roland Jertz¹; Claudia Kriete¹; Matthias Witt¹; Jochen Friedrich¹; Christopher Thompson²; Michael L Easterling³; Eugene N Nikolaev⁴; Goekhan Baykut¹; ¹Bruker Daltonics GmbH, Bremen, Germany; ²Bruker Daltonics Inc., Billerica, MA; ³Bruker Daltonics, Billerica, MA; ⁴The Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia
- TP 438 **A Timing Control Method to Prevent Ion Overtake in a Multi-turn Time-of-Flight Mass Spectrometer (infITOF);** Miki Shinichi¹; Hirofumi Nagao¹; Michisato Toyoda²; ¹MSI, Tokyo, INC., Chofu, Tokyo, Japan; ²Osaka University, Toyonaka, Osaka, Japan
- TP 439 **Improving m/z Resolution in Charge Detection Mass Spectrometry by Reduction of Ion Trap Energy Dependence;** Joanna Hogan¹; Martin F Jarrold¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- TP 440 **A Novel, Miniaturized Linear Wire Ion Trap Mass Analyzer;** Qinghao Wu¹; Yuan Tian¹; Ailin Li¹; Daniel Austin¹; Richard N Zare²; ¹Brigham Young University, Provo, Utah; ²Stanford University, Stanford, CA
- TP 441 **New Analysis of the Bradbury-Nielsen Gates with Space Charge as Applied to Time-of-flight Analyzers;** Robert Jackson; Instrumental Design Physics, LLC, Littleton, MA
- TP 442 **Addressing the 100 Isotope Physics Challenge: Orbitrap Mass Spectrometry as a Means of High-Dimension Clumped and Position-specific Isotope Analysis;** John Eiler¹; Johannes Schwieters²; Dieter Juchelka²; Alexander A Makarov²; Jens Griep-Raming²; ¹California Institute of Technology, Pasadena, CA; ²Thermo Fisher Scientific, Bremen, DE

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- TP 443 **CZE-nanoESI-SLIM-IMS-MS Platform for Comprehensive, Ultrasensitive Proteome Analyses;** Roza Wojcik¹; Ian K Webb¹; Yehia M Ibrahim¹; Derek F Hopkins¹; Spencer A Prost¹; Randolph V Norheim¹; Daniel J Orton¹; Sandilya Garimella¹; Liulin Deng¹; Ahmed M Hamid¹; Ryan T Kelly¹; Erin Baker¹; Richard D Smith¹; ¹PNNL, Richland, WA
- TP 444 **Separation of Protein Conformers by High Resolution Ion Mobility-Mass Spectrometry;** Urs Rohner¹; Michael Groessl¹; Stephan Graf¹; ¹TOFWERK, Thun, Switzerland
- TP 445 **Protein Domain Structure Influences the Collision-Induced Ejection of Small Molecule Binders: Implications for the Development of Pharmaceutical Compounds;** Rachel Martini¹; Joseph Eschweiler¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- TP 446 **Native and Denatured Protein Structural Studies using Ion Mobility MS and Ion Activation Techniques;** Ruwan Kurulugama¹; George C Stafford¹; Joseph Eschweiler²; Brandon T Ruotolo²; John Fjeldsted¹; ¹Agilent Technologies, Santa Clara, CA; ²University of Michigan, Ann Arbor, MI
- TP 447 **MS-based Epitranscriptomics: New Roles for Ion Mobility and Fragmentation Techniques;** Daniele Fabris¹; Rebecca D'Esposito²; Jennifer Lippens²; Michael Miller²; William McIntyre²; Rebecca Rose²; ¹The RNA Institute, University at Albany, Albany, NY; ²The RNA Institute, University at Albany Albany, NY
- TP 448 **Analysis of Native-Like Protein and Protein Complex Ions using Structures for Lossless Ion Manipulations (SLIM);** Samuel J. Allen¹; Rachel M. Eaton¹; Matthew F. Bush¹; ¹University of Washington, Seattle, WA



- TP 449 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Rapidly Detect Subtle Differences in Antibody Glycoforms**; Yuwei Tian¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- TP 450 **Ion Mobility Employed as a Second Dimension Separation of Isomeric Glycoforms in Glycopeptides**; Gege Xu¹; Elisha Goonatilake¹; Jasmine Davis¹; Mariana Barboza¹; Carlito B Lebrilla¹; ¹UC Davis, Davis, CA - California
- TP 451 **Water-Mediated Dimerization of Ubiquitin Ions Captured by Cryogenic Ion Mobility-Mass Spectrometry**; Kelly Servage¹; David H Russell²; ¹Texas A&M University, College Station, Texas; ²Texas A&M University, College Station, TX
- TP 452 **Structural Investigation and Binding Site Determination of Huntingtin Protein/Peptide-ligand Complexes by IMS-HDX-MS/MS and Molecular Dynamics Simulations**; Samaneh Ghassabi Kondalaji¹; Mahdiar Khakinejad¹; Stephen J Valentine¹; Justin Legleiter¹; ¹West Virginia University, Morgantown, WV
- TP 453 **An LC/ESI-IM-MS/MS Assay for Identification and Quantification of Host Cell Proteins in Therapeutic Monoclonal Antibodies**; Catalin Doneanu¹; Brad J Williams²; Ian Morns³; Andrew Borthwick⁴; Jackson Pope⁴; Ying-Qing Yu⁵; Weibin Chen⁵; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA; ³Waters, Newcastle upon Tyne, UK; ⁴Waters, Newcastle upon tyne, UK; ⁵Waters, Milford, MA
- TP 454 **Rapid Profiling of Cellular Extracts using Ion Mobility-Mass Spectrometry**; Brett Harper¹; Brooke Brown¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- TP 455 **Integrating Ion Mobility Separation into Peptide Mapping for Therapeutic Protein Characterization: Qualitative and Quantitative Aspects**; Ying-Qing Yu¹; Liuxi Chen¹; Henry Y Shion¹; Weibin Chen¹; ¹Waters, Milford, MA
- TP 456 **Evaluation of Formulation-Induced Aggregation in Peptide Drug Products by IMS-MS**; Elizabeth E Pierson¹; Nicholas A Pierson¹; Paul L Walsh¹; ¹Merck Research Laboratories, Rahway, NJ
- TP 457 **Investigation of the Interaction between Antimicrobial Peptides and Lipid Membranes Using Ion Mobility Mass Spectrometry Coupled with Isothermal Titration Calorimetry**; Anqi Chen¹; John W Patrick¹; David H Russell¹; ¹Texas A&M, College Station, TX
- TP 458 **Monitoring Conformational Landscape of Prion Protein**; Guillaume Van der Rest¹; Human Rezaei²; Frederic Halgand³; ¹Universite Paris-Sud, Orsay, France; ²INRA, Jouy-en-Josas, France; ³CNRS, Orsay, France
- TP 459 **Structural transitions of Bovine Serum Albumin Studied by IMS-IMS-MS**; Alexander D Jacobs¹; Joseph D Eschweiler²; Sugyan Dixit²; Brandon T Ruotolo²; David E Clemmer¹; ¹Indiana University, Bloomington, IN; ²University of Michigan, Ann Arbor, MI
- TP 460 **Characterization of Cytochrome c Intramolecular Interactions using nanoESI-HDX-TIMS-MS and Molecular Dynamics**; Juan Camilo Molano¹; Khoa Pham¹; Jaroslava Miksovska¹; Mark E Ridgeway²; Melvin Park²; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL; ²Bruker Daltonic, Billerica, MA
- TP 461 **Effects of Chain Length on the cis/trans Isomerization Mediated Folding of Polyproline Helices**; Daniel W Woodall¹; Tarick J El-Baba¹; David E Clemmer¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- TP 462 **Introduction of Hydrophilic Sites: How Physical Modifications Alter the Conformer Preferences of Gramicidin A**; John Patrick¹; David H Russell²; ¹Texas A&M, college station, TX; ²Texas A&M University, College Station, TX
- TP 463 **Characterization of Kinetically Trapped Intermediates of Microperoxidase-11 using TIMS-MS/MS and Molecular Modeling**; Jacob Porter¹; Alyssa Garabedian¹; Paolo Benigni¹; Jaroslava Miksovska¹; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL
- TP 464 **Proline Influences the Binding of Zinc to Oxytocin**; Daniel R. Fuller¹; Matthew S. Glover¹; DoYong Kim²; David H. Russell²; David E. Clemmer¹; ¹Indiana University, Bloomington, IN; ²Texas A&M University, College Station, TX
- TP 465 **Determination of the Gas-Phase Energy Landscape of Substance P by IMS-IMS-MS**; Chris Conant¹; David H Russell²; David E Clemmer¹; ¹Indiana University, Bloomington, IN; ²Texas A&M, College Station, TX
- TP 466 **Analysis of Ionic Self-Complementary Peptides by Ion Mobility Spectrometry-Mass Spectrometry**; Zhichao Zhang¹; Daniel R. Fuller¹; Tarick John El-Baba¹; David E Clemmer¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- TP 467 **Comparison of Ion Mobility and Capillary Electrophoresis Mass Spectrometry Techniques for Cysteine Connectivity Identification of Peptides Bearing Intra-Molecular Disulfide Bonds**; Philippe Massonnet¹; Cédric Delvaux²; Gregory Upert³; Jean R. N. Haler¹; Jan Jordens⁴; Maarten Honing⁴; Ynze Mengerink⁴; Johann Far¹; Nicolas Gilles³; Loic Quinton¹; Edwin De Pauw¹; ¹University of Liège, Liège, Liège; ²Laboratory of Mass Spectrometry - ULg, Liege, Belgium; ³CEA, DSV/iBiTec - S/SIMOPRO, Gif-sur-Yvette, France; ⁴DSM Resolve, Geleen, The Netherlands
- TP 468 **Using Gas Phase Conformations to Understand the Role of Solvent in Establishing Biomolecule Structure in Solution**; Tarick El-Baba¹; Daniel Fuller¹; DoYong Kim²; Dylan Rogers³; Faizan Khan³; David A Hales³; David H Russell²; David E Clemmer¹; ¹Indiana University Dept. Chemistry, Bloomington, IN; ²Texas A&M, College Station, TX; ³Hendrix College, Conway, AR
- TP 469 **Separation of Isomers in Lipidomics and Metabolomics Experiments by High Resolution Ion Mobility-Mass Spectrometry**; Michael Groessl¹; Stephan Graf¹; ¹TOFWERK, Thun, Switzerland
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- TP 472 **Evaluating Effects of Metagenome Database Quality and an Optimized LC/LC-MS/MS Approach for Obtaining Deeper Proteome Coverage of Complex Microbial Communities**; Ramsunder Iyer^{1,2}; Richard J Giannone²; Rose S Kantor³; Susan T.L Harrison⁴; Robert J Huddy⁴; Jillian F Banfield⁵; Robert L Hettich²; ¹Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN; ²Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; ³Department of Plant and Microbial Biology, University of California, Berkeley, CA; ⁴Centre for Bioprocess Engineering Research, Department of Chemical Engineering, University of Cape Town, Cape Town, South Africa; ⁵Department of Earth and Planetary Sciences, University of California, Berkeley, CA
- TP 473 **Universal Derivatization of Metabolites for Improved Sensitivity in LC-MS**; James Edwards; Saint Louis University, St Louis, MO



- TP 474 **Optimization of Size Exclusion Chromatography and Atmospheric Pressure Ionization Enabling Characterization of Intact Lignin and Its Degradation Products;** Anastasia Artemyeva¹; Kubatova Alena¹; Evguenii I. Kozliak¹; ¹University of North Dakota, Grand Forks, ND
- TP 475 **Characterization of Electrochemically Decomposed Lignin Using Liquid Chromatography-High Resolution Mass Spectrometry;** Tobias Dier¹; Sarah Henrikus¹; Verlaïne Fossog¹; Rolf Hempelmann¹; Dietrich A Volmer¹; ¹Saarland University, Saarbrücken, Germany
- TP 476 **Deeper Proteomics using Actively Modulated Online HILIC×nRPLC-HRMS;** Andrea Gargano^{1,2}; Martin Samonig³; Michael Woldergebrüel²; Remco Swart³; Garry Corthals⁴; Peter Schoenmakers²; ¹VU University Amsterdam, Amsterdam, Netherlands; ²University of Amsterdam, Amsterdam, The Netherlands; ³Thermo Fisher Scientific GmbH, Germering, Germany; ⁴University of Amsterdam, Amsterdam, NL
- TP 477 **Low-Temperature Mobile Phase for Peptide Trapping at Elevated Separation Temperature Prior to Nano RP-HPLC-MS/MS;** Matthias Schöbinger¹; Oskar-James Klein¹; Goran Mitulovic²; ¹Medical University of Vienna, Clinical Institute of Laboratory Medicine, Wien, Austria; ²Medical University of Vienna, KIMCL, Vienna, No State/Province
- TP 478 **Porous Graphitic Carbon Packed Capillaries for the LC-MS/MS Analysis of RNA Modified Nucleosides;** Robert Ross¹; Peter Sarin²; Hannes Drexler²; Sebastian Leidel²; Patrick A Limbach¹; ¹University of Cincinnati, Cincinnati, OH; ²Max Planck Institute for Molecular Biomedicine, Munster, Deutschland
- TP 479 **Redesign of Peptide Mapping Gradients to Resolve Complex Biological Samples;** Xinli Yang; Rosalind Franklin University, North Chicago, IL
- TP 480 **LC/MS/MS Method for the Determination of Tricyclic and Tetracyclic Antidepressants in Human Urine;** Amber Awad¹; Kendra Parker¹; Lawrence Andrade²; ¹Dominion Diagnostics, N. Kingstown, RI; ²Dominion Diagnostics, North Kingstown
- TP 481 **A Fast and Sensitive Chiral LC-MS/MS Assay for Ketamine and its Metabolites in Human Plasma;** Michel Coutu¹; Evgueni Fedorov¹; Jean-François Larocque¹; Simon Bourgeois¹; ¹Biotrial Bioanalytical Services, Laval, QC
- TP 482 **Proteomics Needs Better Chromatography;** Evgenia Shishkova¹; Alexander S Hebert²; Michael S Westphall²; Joshua J Coon²; ¹JJ Coon Research Group, Madison, Wisconsin; ²University of Wisconsin-Madison, Madison, WI
- TP 483 **A Novel Approach to Studying Thiamine Kinetics: an LC/ESI-MS/MS-based Method for the Analysis of Thiamine and Derivatives in Biological Samples;** Jaeah Kim¹; Jason Zastre¹; Michael G Bartlett¹; ¹University of Georgia, Athens, GA
- TP 484 **A Functional Group Approach to Determining the Effects of Mobile Phase Modifiers on the Negative Ion ESI Ionization Efficiency;** Melanie Odenkirk¹; Stephen Lucas¹; Christine A. Hughey²; ¹James Madison University, Harrisonburg, VA; ²James Madison University, Harrisonburg, VA
- TP 485 **A Fast LC/MS/MS Method for High Sensitivity Determination of 24 Perfluorocompounds in Textiles;** Jun Xiang Lee¹; Zhe Sun¹; Jie Xing¹; Zhaoqi Zhan¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore
- TP 486 **Exploring the Effects of Alternative Dynamic Exclusion Algorithms on Peptide Identification Experiments;** Nina Soltero¹; Graeme C McAlister¹; Derek Bailey¹; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 487 **Targeted Profiling of Oxylipins and Endocannabinoids in Biological Samples using the Nanoflow ionKey/MS system – Method Development and Validation;** Sandra Gouveia-Figueira¹; Malin Linder Nording¹; ¹Umea University, Umea, SE
- TP 488 **The Simultaneous Detection of a Panel of Drugs of Abuse in Post-mortem Hemolyzed Blood Samples (n=40) by LC-ESI-laminar Flow MS/MS;** Sabra Botch-Jones¹; Raquel LeBlanc¹; ¹Boston University School of Medicine, Boston, MA
- TP 489 **UHPLC Optimization Study for Improved LC-MS Performance and Throughput;** Martin Ruehl; Thermo Fisher Scientific, Germering, Germany
- TP 490 **A Study of the γ-Radiolysis of Di-Dodecyl Di-Octyl Diglycolamide (D3DODGA) using UHPLC-ESI-MS Analysis;** Kristyn M Johnson¹; Christopher A Zarzana¹; Gary S Groenewold¹; Bruce J Mincher¹; Andreas Wilden²; Holger Schmidt²; Giuseppe Modolo²; Beatrix Santiago-Schübel³; ¹Idaho National Laboratory, Idaho Falls, ID; ²Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung- Nukleare Entsorgung und Reaktorsicherheit, Jülich, Germany; ³Forschungszentrum Jülich GmbH, Zentralinstitut für Engineering, Elektronik und Analytik, Jülich, Germany
- TP 491 **The Use of a HILIC Peptide Retention Prediction Model to Predict the Presence of Modifications in Histones;** Majors Badgett¹; Barry Boyes²; Ron Orlando¹; ¹The University of Georgia, Athens, GA; ²Advanced Materials Technology, Wilmington, DE
- TP 492 **Automation and Remote Visualization of Screening Data;** David M Cox¹; Burkhard Schaefer²; John Gibbons³; Viktor Iassinskii³; ¹SCIEX, Concord, ON; ²BSSN Software, Darmstadt, Germany; ³SCIEX, Concord, ON
- TP 493 **Long Term Test on a New Four-Channel HPLC;** Pengxiang Yang¹; BC cha¹; Terry N Olney¹; John Brann²; Christopher Elicone²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Franklin, MA
- TP 494 **New Supercharging Agents for TFA-Based LC-MS of Peptides and Proteins;** Michael Nshanian¹; Rachel Loo²; Joseph A Loo²; ¹University of California Los Angeles, Los Angeles; ²UCLA, Los Angeles, CA
- TP 495 **Matrix Effects: Do They Differ between SFC/ESI-MS and LC/ESI-MS?** Alfred Svan¹; Mikael Hedeland^{1,2}; Torbjörn Arvidsson^{1,3}; Curt E Pettersson¹; ¹Uppsala University, Uppsala, Sweden; ²National Veterinary Institute (SVA) Dept. of Chemistry, Environment and Feed Hygiene, Uppsala, Sweden; ³Medical Products Agency, Uppsala, Sweden
- TP 496 **Development of a Novel Nano Separation Device for Robust and Accurate Gradient Delivery with Intelligent Diagnostics;** Ole Bjeld Hørning¹; Stephanie Kaspar-Schoenefeld²; Christoph Gebhardt²; Peter Aagaard Nielsen¹; Alexandre Podtelejnikov¹; Michael Barrett Andersen¹; Nicolai H Bache¹; ¹Bruker Daltonics Scandinavia, Odense, Denmark; ²Bruker Daltonik GmbH, Bremen, Germany
- TP 497 **HILIC and Mixed-Mode Retention of the FluoroPhenyl Stationary Phase;** Shun-Hsin Liang¹; Carroll Frances¹; Sharon Lupo¹; Ty Kahler¹; ¹Restek Corporation, Bellefonte, PA
- TP 498 **Method and Software Workflow for Integrating Paired CE-MS and LC-MS Bottom-up Proteomics Data from SDS-PAGE Pre-fractionated Samples;** Yassene Mohammed^{1,2}; Anthonius A. M. Heemskerck¹; Dana Ohana¹; Hans Dalebout¹; André M Deelder¹; Oleg Mayboroda¹; Magnus Palmblad¹; ¹LUMC, Center for Proteomics and Metabolomics Leiden, NL; ²UVic - Genome BC Proteomics Centre, Victoria, Canada

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- TP 500 **Integrated Software for Data Processing and Analysis in Direct Infusion Ultra-High Resolution / Accurate Mass Spectrometry Based 'Top-Down' Lipidomics Workflows;** Yasuto Yokoi¹; Yukihiro Fukamachi¹; David Peake²; Reiko Kiyonami²; Eileen Ryan³; Gavin E Reid³; ¹Mitsui Knowledge Industry Co, Tokyo, Japan; ²Thermo Fisher Scientific, San Jose, CA; ³University of Melbourne, Victoria, Australia
- TP 501 **A Lipid Mass Spectral Library for Human Plasma;** Paul D Hutchins¹; Dain R Brademan^{2,3}; Jason W Russell⁴; Michael S Westphall²; Joshua J Coon^{2,3,5}; ¹University of Wisconsin Madison, Madison, Wisconsin; ²Genome Center, University of Wisconsin, Madison, WI; ³Department of Chemistry, University of Wisconsin, Madison, WI; ⁴Morgridge Institute for Research, Madison, WI; ⁵Biomolecular Chemistry, University of Wisconsin, Madison, WI
- TP 502 **SimLipid: Software Platform for Automating Shotgun, LC-MS and MALDI-MS Based High-Throughput Lipidomics;** Ningombam Sanjib Meitei¹; Himani Gupta¹; Arun Apte²; ¹PREMIER Biosoft, Indore, India; ²PREMIER Biosoft, Palo Alto, CA
- TP 503 **Structural Characterization of Membrane Glycolipids from Marine Sponge-associated Bacteria by Mass Spectrometry;** Benjamin L Oyler¹; Courtney E Chandler²; Fan Zhang³; Christopher J Thompson⁴; Jeremy J Wolff⁴; Michael L Easterling⁴; Robert K Ernst²; Russell T Hill³; David R. Goodlett²; ¹University of Maryland, Baltimore, Whiteford, MD; ²University of Maryland, Baltimore, Baltimore, MD - Maryland; ³University of Maryland Center for Environmental Science, Baltimore, MD - Maryland; ⁴Bruker Daltonics, Billerica, MA
- TP 504 **Identification and Quantitation of Unsaturated Glycerolipids from Human Plasma using the Paternò-Büchi Reaction and Tandem Mass Spectrometry;** Hilary Brown¹; Yu Xia¹; ¹Purdue University, West Lafayette, IN
- TP 505 **Study and Optimization of online Paternò-Büchi Reactions for Structural Analysis of Unsaturated Lipids using Mass Spectrometry;** Xiaoxiao Ma^{1,2}; Pei Su¹; Zheng Ouyang^{1,2}; Yu Xia²; ¹Purdue University-Weldon School of Biomedical Engineering, West Lafayette, IN; ²Purdue University-Department of Chemistry, West Lafayette, IN
- TP 506 **Top-down Structural Elucidation of Gram-negative Bacterial Endotoxins by Tandem Mass Spectrometry;** Mohd M. Khan¹; Benjamin L Oyler²; Kelsey A. Gregg³; Robert K. Ernst³; Alan S. Cross⁴; David R Goodlett²; ¹University of Maryland School of Pharmacy, Baltimore, MD; ²Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD; ³Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, MD; ⁴Center for Vaccine Development, University of Maryland School of Medicine, Baltimore, MD
- TP 507 **Structural Characterization of Lipid Biomarkers from Staphylococcus aureus following Microextraction for Mass Spectrometric Phenotyping;** Lisa Leung¹; Benjamin Oyler²; Robert Ernst³; David R Goodlett²; ¹University of Maryland, Baltimore, MD; ²University of Maryland School of Pharmacy, Baltimore, MD; ³University of Maryland Baltimore, Baltimore, MD
- TP 508 **N-Succinylation of L-lysyl-phosphatidylglycerol in Bacillus subtilis;** Paulos Chumala¹; Metin Atila¹; George Katselis¹; Yu Luo²; ¹University of Saskatchewan, Saskatoon, Canada; ²University of Saskatchewan, Saskatoon, SK
- TP 509 **Systematic Fragmentation of Lipid A Variants by Multiple and Hybrid MS/MS Techniques;** Christopher Martin Crittenden¹; William Ryan Parker¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TP 510 **In-situ Characterization of Phospholipids Mixture on Tissue Sections using Wide Ion Gate HE-CID Experiment and ASDF MS/MS Spectra;** Simona Salivo¹; Yuzo Yamazaki²; Peter Quinto Tranchida¹; Luigi Mondello¹; Omar Belgacem³; ¹University of Messina, Messina, Italy; ²Shimadzu Corporation, Kyoto, Japan; ³Shimadzu, Kratos Manchester, United Kingdom
- TP 511 **Using MS/MS and MSn to Distinguish Cytotoxic J-series Prostaglandin Isomers Produced in Tumorigenic Keratinocytes;** Robert Kobet¹; Rukiyah T. Van Dross¹; Allison S. Danelli¹; ¹East Carolina University, Greenville, NC
- TP 512 **Conformational Atlas of 7 Classes of Sphingolipids and Glycerophospholipids Mapped by Ion Mobility-Mass Spectrometry;** Katrina L. Leaptrot¹; Jody C. May¹; James N. Dodds¹; John A. McLean¹; ¹Vanderbilt Dept. of Chemistry, Nashville, TN
- TP 513 **Differentiation of Triacylglycerol Regioisomers Using Differential Ion Mobility Spectrometry;** Jinyuan Wang¹; Larry J Campbell²; Paul RS Baker¹; ¹SCIEX, Redwood City, CA; ²SCIEX, Concord, ON
- TP 514 **Identification of Lipid Metabolites of Docosahexaenoic and Arachidonic Acids in Human Blood Using Stable Isotope Labeled Compounds;** Karl R Kevala¹; Mark Sanders²; Hee-Yong Kim¹; ¹National Institutes of Health, Bethesda, MD; ²Thermo Fisher Scientific, Somerset, NJ
- TP 515 **Identification and Characterization of Sulfolipids Found in Nitzschia palea;** Larry Sallans¹; Daniel Betz²; Stephen F Macha²; Edna S. Kaneshiro²; ¹University of Cincinnati, Cincinnati, OH; ²University of Cincinnati, Cincinnati, OH
- TP 516 **Role of pH and Mobile Phase Modifiers on Untargeted RP LC-MS Analysis of Lipid Extracts;** Elena Sokol¹; David Peake²; ¹Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ²Thermo Fisher Scientific, San Jose, CA
- TP 517 **Identification of Metabolites of Novel Sphingoid Bases in Sphingolipid-depleted Cells using Liquid-Chromatography Electrospray Tandem Mass Spectroscopy;** Brandon M Kenwood¹; Samuel Kelly¹; Jingjing Duan¹; Alfred H Merrill Jr¹; Cameron Sullards¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 518 **Identification of a Novel Lipid Family Containing a Modified Head Group;** Seetaramanjaneyulu Gundimeda¹; Arunkumar Padmanaban²; ¹Agilent technologies, bangalore, karnataka; ²Agilent technologies, Bangalore, India

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- TP 520 **Determination of Selectivity Influenced by Liquid-Liquid Extraction in Global Metabolomics using UHPLC-qTOF-MS;** Albert Elmsjö¹; Mikael Karl Robert Engskog²; Jakob Haglöf¹; Torbjörn Arvidsson^{1,3}; Curt Pettersson¹; ¹Department of Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; ²Department Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; ³Medical Product Agency, Uppsala, Sweden

- TP 521 **Widely Targeted Analysis of Hydrophilic Anionic Metabolites in Mammalian Cells by Ion Chromatography Coupled with High Resolution Mass Spectrometry;** Yoshihiro Izumi¹; Takahiro Suzuki²; Motokazu Kimura²; Shigeru Sakamoto²; Takeshi Bamba³; ¹Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; ²Thermo Fisher Scientific Japan, Tokyo, Japan; ³Medical Institute of Bioregulation, Kyushu Univ. Fukuoka, Japan
- TP 522 **Systematic Assessment and Selection of Liquid and Solid-Phase Methods in the Design of Sequential Extraction Protocols for LC-MS Based Metabolomics;** Dmitri Sitnikov¹; Cian S Morin¹; Dajana Vuckovic¹; ¹Concordia University, Montreal, Canada
- TP 523 **Super-Omics: Liquid-Liquid Extraction for Proteomics, Lipidomics and Metabolomics from a Single Sample, Towards a Method for Biopsies;** Susanne Breittkopf¹; Min Yuan¹; Gerburg Wulfi^{1,2}; John M Asara^{1,2}; ¹Beth Israel Deaconess Medical Center, Boston, MA; ²Harvard Medical School, Boston, MA
- TP 524 **Detection Enhancement of Small Molecules, Lipids and Peptides by Functionalizing Silicon Nanopost Arrays with Fluorous Monolayers;** Heather Anderson¹; Nicholas Morris¹; Matthew Powell¹; Trust T Razunguzwa¹; ¹Protea Biosciences, Morgantown, WV
- TP 525 **A Real-time Analysis of Brain Energy Metabolism by Micro-dialysis Linked Ion Chromatography-MS;** Yuki Sugiura; Keio University, Tokyo
- TP 526 **Characterizing Temporal And Inter-Individual Functional Differences in Infant Gut Microbiome by a Metaproteomics Approach;** Weili Xiong¹; Michael Morowitz²; Jillian Banfield³; Robert Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Pittsburgh, Pittsburgh, PA; ³University of California, Berkeley, CA
- TP 527 **Custom isotopic N,N-Dimethyl Leucine (iDiLeu) Reagents Enable Absolute Quantification of Amine-containing Metabolites and Its Application to Human Cerebrospinal Fluid;** Pingli Wei¹; Ling Hao²; Jingxin Wang²; Xuefei Zhong¹; Lingjun Li²; ¹University of Wisconsin Madison, Madison, Wisconsin; ²University of Wisconsin Madison, Madison, WI
- TP 528 **Sub-Minute, Comprehensive Metabolomics Measurements for Disease and Exposure Research;** Xing Zhang¹; Michelle V Romm²; Erika M Zink³; Daniel J Orton³; Yehia M Ibrahim³; Matthew E Monroe³; Justin G Teeguarden³; Thomas O Metz³; Richard D Smith³; Nichole A Reisdorff¹; Erin S Baker³; ¹Anschutz Medical Campus, University of Colorado Denver, Aurora, CO; ²Agilent Technologies, Santa Clara, CA; ³Pacific Northwest National Lab, Richland, WA
- TP 529 **Online-SPE-HILIC-ESI-MS Analysis of Redox Cofactors in Chlamydomonas Reinhardtii Algae Cells;** Alexander Schriewer¹; Heiko Hayen¹; ¹Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany
- TP 532 **Metabolic Phenotyping of Cell Lines by Rapid Evaporative Ionization Mass spectrometry;** Emrys Jones¹; Emmanuelle Claude¹; James Langridge¹; Fiona Henderson²; Adam W McMahon²; Zoltan Takats³; Steve Pringle¹; ¹Waters Corporation, Wilmslow, UK; ²Wolfson Molecular Imaging Centre, Manchester, UK; ³Imperial College London, South Kensington Campus London, United Kingdom
- TP 533 **Metabolomic Profiling in Pulmonary Arterial Hypertension Disease Models;** David P Marciano¹; Caiyun grace Li¹; Jan k Hennigs¹; Marlene Rabinovitch¹; Michael Snyder¹; ¹Stanford University School of Medicine, Palo Alto CA, USA
- TP 534 **Non-targeted Metabolite Profiling and Antioxidant Activity of Genetically Diverse Soybean Seeds;** Yongsoo Choi¹; Jiuliang Xu²; Jeong-Sook Shin¹; Jung-Kyung Moon³; ¹Korea Institute of Science and Technology, Gangneung, South Korea; ²Korea Institute of Science and Technology, Geogneung, South Korea; ³National Institute of Crop Science, Cheongju-Si, Chungbuk
- TP 535 **Identification and Chemical Characterization of Marine Natural Products Using UPLC-QTOF-MS Coupled to a Novel Informatics Platform;** Roger G. Linington¹; Kenji L. Kurita¹; Jimmy Yuk²; Kate Yu²; Mark Wrona²; Giorgis Isaac²; ¹Simon Fraser University, Burnaby, BC, Canada; ²Waters Corporation, Milford, MA
- TP 536 **Isotopic Ratio Outlier Analysis (IROA) Global Metabolome Interrogation of an Actinomycete Bacterium following Introduction of a Novel Pathway;** Felice de Jong¹; Taylor A. Lundy²; Christopher W W Beecher^{1,3}; Amy L Lane²; ¹IROA Technologies LLC, Bolton, MA; ²University of North Florida, Jacksonville, FL; ³University of Florida, Gainesville, FL
- TP 537 **Increasing Arginine Production in C. Glutamicum by Rational Strain Design and Discovery Metabolomics: Linking HRAM QTOF Data to Biology;** Frederik Walter¹; Marcus Persicke¹; Aiko Barsch²; Christian Ravensborg³; Heiko Neuweger²; Matthias Szesny²; Nikolas Kessler²; Jörn Kalinowski¹; ¹Bielefeld University, Bielefeld, Germany; ²Bruker Daltonics Ltd, Bremen, Germany; ³Bruker Daltonics, Bremen, Germany
- TP 538 **Metabolite Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDchips;** Christopher George¹; Haddon Goodman¹; Gregory Boyce¹; ¹Protea Biosciences, Morgantown, WV
- TP 539 **Environmental Exposure to Ionizing Radiation Induces Dysbiosis in Gut Microbiome and Fecal Metabolome;** Maryam Goudarzi¹; Jonathan Jacobs²; Tytus Mak³; Bo-Hyun Moon⁴; Steve Strawn⁴; Jonathan Braun²; David Brenner⁵; Albert Fornace Jr⁴; ¹Georgetown University, Washington DC, DC; ²UCLA, Los Angeles, CA; ³NIST, Rockville, MD; ⁴Georgetown University, Washington, DC; ⁵Columbia University, New York, NY
- TP 540 **Abiotic Stresses Influence Organic Metabolite Profiles in Soils Hosting Populus Trees and a Microbial Community;** Charles J. Doktycz¹; Collin M. Timm¹; Keiji G Asano¹; David J Weston¹; Dale A. Pelletier¹; Greg Hurst¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- TP 541 **Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway;** Loren Y Olson¹; Baljit Ubhi¹; ¹SCIEX, Redwood City, CA
- TP 542 **Untargeted Metabolomics with Fungal Artificial Chromosomes (FAC-MS) Allows Discovery and Facile Dissection of Natural Product Biosynthesis;** Kenneth D Clevenger¹; Jin Woo Bok²; Rosa Ye³; Galen P Miley¹; Thomas Velk²; Cynthia Chen³; KaHoua Yang²; Peng Gao¹; Matthew Lamprecht³; Paul M Thomas¹; Md Islam³; Chenggang C Wu³; Nancy P Keller²; Neil L Kelleher¹;

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- TP 530 **Rapid Detection of Pathogenic Amoeba in Water Distribution Systems using UPLC-MS;** Zhihao Yu¹; Haylea Miller²; Geoffrey Puzon²; Brian H Clowers¹; ¹Washington State University, Pullman, WA; ²CSIRO Land and Water, Perth, Australia
- TP 531 **Metabolomic evaluation of conditions favoring mycotoxin production in isolates of Fusarium fungi;** Mark Busman; USDA, ARS, NCAUR, BFP, Peoria, IL

- ¹Northwestern University, Evanston, IL; ²University of Wisconsin Madison, Madison, Wisconsin; ³Intact Genomics, Inc, St. Louis, MO
- TP 543 **In vivo Analysis of Metabolites in Single Embryonic Cells in the Developing Frog (Xenopus) Embryo using Microcapillary-Sampling CE-ESI-MS;** Erika Portero¹; Rosemary M Onjiko¹; Sally A Moody¹; Peter Nemes¹; ¹The George Washington University, Washington, DC
- TP 544 **Eavesdropping on Marine Microbial Communication: Influence of Quorum Sensing on the Vibrio campbellii Metabolome;** Gregory Ellis¹; Brian J. Eddie²; Arnaldo A. Torres Padua³; W. Judson Hervey IV⁴; Gary J. Vora⁴; Dagmar H. Leary⁴; ¹National Research Council NRL Fellow, Washington, DC; ²American Society of Engineering Education NRL Fellow, Washington, DC; ³University of Puerto Rico Mayaguez, Mayaguez, PR; ⁴Center for Bio/Molecular Science and Engineering, Naval Research Laboratory, Washington, DC
- TP 545 **Untargeted 2-Sample-Comparison using High-Resolution Data from LC/Ion Mobility Q-TOF Mass Spectrometers via a Novel 4D Molecular Feature Extraction Algorithm;** Frank Kuhlmann¹; Xiangdong Li¹; Ed Darland¹; ¹Agilent Technologies, Santa Clara, CA
- TP 546 **Metabolic Profiling of Strawberry Leaves Infected by Xanthomonas Fragariae using UPLC/QTOF Mass Spectrometry;** Min-Sun Kim¹; Geum-Sook Hwang²; ¹Korea Basic Science Institute, Seoul, Republic of Korea; ²Korea Basic Science Institute, Seoul, Republic of Korea
- TP 547 **Global Metabolomics Approach to Identify Pathways Effected by Glyphosate in Yeast;** Gregory Boyce¹; Mark Szewc¹; ¹Protea Biosciences, Morgantown, WV
- TP 548 **Chemical Profiling of Actaea Species and Commercial Products using UPLC-QToF-MS;** Jimmy Yuk¹; Maged Sharaf²; Kate Yu¹; Mark Wrona¹; Giorgis Isaac¹; ¹Waters, Milford, MA; ²American Herbal Products Association, Silver Spring, MD
- TP 549 **Non-targeted Differential Screening using LC-HRAM-MS as a Tool for Evaluating Differences in Chemical Composition between Samples and Sample Groups;** Daniel Arndt¹; Arno Knorr¹; Mark Bentley¹; ¹Philip Morris International R&D, Neuchâtel, Switzerland
- TP 550 **Non-targeted Differential Screening of Complex Matrices using GC×GC-TOFMS for Comprehensive Characterization of Chemical Composition and Determination of Significant Differences;** Martin Almstetter¹; Arno Knorr¹; Quentin Dutertre¹; Elyette Martin¹; Antonio Castellon¹; Pavel Pospisil¹; Mark Bentley¹; ¹Philip Morris International, Neuchâtel, Neuchâtel
- TP 551 **Atmospheric Pressure Gas Chromatography Mass Spectrometry (APGC-MS) Based Metabolomics Profiling of Grape Volatiles;** Manoj Ghaste^{1,2}; Giuseppe Astarita³; Fulvio Mattivi²; Vladimir Shulaev¹; ¹University of North Texas, Denton, TX; ²Fondazione Edmund Mach, San Michele all'Adige TN, Italy; ³Waters, Milford, MA
- TP 552 **Comparison of Direct Introduction on Orbitrap Fusion and FT-ICR at High-end Resolution for Global Metabolite Screening;** Ulli Martin Hohenester^{1,2}; Pierre Barbier Saint Hilaire¹; Benoît Colsch¹; Francois Fenaille¹; Jean-claude Tabet¹; Christophe Junot¹; Richard B Cole²; ¹Commissariat à l'énergie atomique et aux énergies alternatives, Gif Sur Yvette Cedex, Fr; ²Sorbonne Universités, UPMC Univ Paris 06, Institut Parisien de Chimie Moléculaire, Paris, Fr
- TP 553 **Development of High-Performance Chemical Isotope Labeling LC-MS for Profiling Alcoholic Hydroxyl-Containing Metabolites in Metabolomics;** Shuang Zhao¹; Liang Li¹; ¹Department of Chemistry, University of Alberta, Edmonton, AB, Canada
- TP 554 **Metabolomic Profiling of Food Diets Using Ion Chromatography with High Resolution Orbitrap Mass Spectrometry;** Terri Christison¹; JUNHUA WANG²; Linda Lopez¹; Ralf Tautenhahn³; ¹Thermo Fisher Scientific Inc, Sunnyvale, CA; ²Thermo Fisher Scientific Inc, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA
- TP 555 **Metabolic Profiling of Bladder Cancer Cell Lines Reveals Molecular Alterations Involved in Methylation and Novel Epigenetic Phenotype;** Feng Jin¹; Rashmi Krishnapuram¹; Franklin Gu¹; Salil Kumar Bhowmik¹; Suman Maity¹; Mohan Manikkam¹; Friedrich-Carl von Rundstedt¹; Vasanta Putluri¹; Yair Lotan²; Jonathan Levitt¹; Seth P. Lerner¹; Cristian Coarfa¹; Benny Abraham Kaiparettu¹; Arun Sreekumar¹; Nagireddy Putluri¹; ¹Baylor College of Medicine, Houston, TX; ²University of Texas Southwestern Medical Center, Dallas, TX
- TP 556 **Metabolomic Signatures in Sera from Early Stage Ovarian Cancer Patients;** David A Gaul¹; Christina M Jones¹; Tran Q Long¹; John F McDonald¹; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 557 **Discovery of Altered Metabolic Pathways in PARPi-Resistant Ovarian Cancer;** Chandra Shekar R Ambati¹; Sachin Kumar Gupta¹; Sajna A Vithayathil¹; Suman Maity¹; Laising Yen¹; Benny Abraham Kaiparettu¹; Cristian Coarfa¹; Nagireddy Putluri¹; ¹Vivekananda Shetty¹; ¹Baylor College of Medicine, Houston, TX

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- TP 558 **RNA Modification Mapping - Software Development;** Ningxi Yu¹; Patrick A Limbach¹; ¹University of Cincinnati, Cincinnati, Ohio
- TP 559 **Development of a Computational Algorithm to Predict Mobile Phase Additives for Optimal LC-MS Sensitivity of Oligonucleotides;** Babak Basiri¹; Michael G Bartlett¹; ¹University of Georgia, Athens, GA
- TP 560 **A Flow Injection Inductively Coupled Plasma Mass Spectrometry Method for Quantification of Modified Oligonucleotides;** Fanyu Meng¹; Qiang Tu²; Erin Guidry²; ¹Merck & Co., Inc, Rahway, NJ; ²Merck, Darmstadt, Germany
- TP 561 **Comparison of Q-ToF, Q-Exactive and Triple Quad for Quantitative Bioanalysis of Oligonucleotide Therapeutics;** Yuhuan Ji¹; Qian Liu¹; Qian Li¹; Chengjie Ji¹; Laixin Wang¹; ¹NovaBioAssays, LLC, Woburn, MA
- TP 562 **A Micro-SPE-LC/MS/MS Quantitative Assay for Phosphorodiamidate Morpholino Oligomer (PMOplus®) AVI-7288 in Human Plasma;** Aihua Liu¹; Jianbo Zhang²; Qian Guo¹; Bryce Ashby¹; Scott Reuschel¹; Jay S. Charleston²; Joe Rutkowski²; Min Meng¹; ¹Covance, Salt Lake City, UT; ²Sarepta Therapeutics, Cambridge, MA
- TP 563 **Determination of a 15-mer Antisense Oligonucleotide in Mouse Plasma by LC-MS/MS;** Lili Xing¹; Ying Han¹; Yi Tao¹; Xinping Fang¹; Xin Zhang¹; ¹WuXi AppTec Co., Shanghai, CHINA
- TP 564 **A Sensitive Liquid Chromatogram/Mass Spectrometry Method for the Determination of a Therapeutic siRNA in Human Plasma;** Pei Li¹; Dawei Zhou¹; Xinping Fang¹; ¹WuXi AppTec Co., Plainsboro, NJ
- TP 565 **LC-MS/MS-based DNA Adduct Quantification for Assessing the Etiology and Prevention of Skin Cancer;** Yuxiang Cui¹; Yinsheng Wang²; ¹University of California, Riverside, Riverside, California; ²University of California, Riverside, Riverside, CA
- TP 566 **Differential Mass Spectrometry Analysis of Transfer RNA by Stable Isotope Labelling;** Mellie Paulines¹; Patrick A Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- TP 567 **Evaluating the Specificity of RNase U2 Variants By Mass Spectrometry;** Beulah Mae Ann Solivio¹; Ningxi

- Yu²; Balasubrahmanyam Addepalli²; Patrick A Limbach²; ¹University of Cincinnati, Cincinnati, Ohio; ²University of Cincinnati, Cincinnati, OH
- TP 568 **Screening for Inflammation-induced DNA Adducts with a Comprehensive High Resolution LC-MS3 adductomic Approach**; Andrea Carra¹; Peter W Villalta¹; Romel P Dator¹; Silvia Balbo¹; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN
- TP 569 **Identification of Isomeric Mono-Methylated Nucleosides in Ribonucleic Acids by Liquid Chromatography – Highly Accurate Tandem Mass Spectrometry**; Hiroshi Nakayama¹; Yoshio Yamauchi²; Masato Taoka²; Toshiaki Isobe²; ¹RIKEN Center for Sustainable Resource Science, Wako, Japan; ²Tokyo Metropolitan University, Tokyo, Japan
- TP 570 **Labeling tRNA Digestion Products using polyA Polymerase and Azido-modified NTPs**; Kayla Borland¹; Patrick A Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- TP 571 **High-Resolution/Accurate-Mass LC-MS3 Screening and SRM Relative Quantitation of DNA Adducts as Biomarkers of Drug Susceptibility**; Alessia Stornetta¹; Peter W Villalta²; Stephen S Hecht²; Silvia Balbo²; Shana J Sturla¹; ¹ETH Zurich, Switzerland, CH; ²Masonic Cancer Center, University of Minnesota, Minneapolis, MN
- TP 572 **Interaction of Antitumor Metalloenes with Nucleic Acids**; Rahel Patricia Eberle¹; Stefan Schürch¹; ¹University of Bern, Bern, Switzerland
- TP 573 **Characterization of Amino Acid-Linked Platinum Complexes and Their Adducts to RNA Using Tandem Mass Spectrometry Approaches**; M. T. Rodgers¹; C. C. Hech¹; L. Hamlow¹; Y. Zhu¹; H. Roy¹; S. Strobehn¹; B. Kimuntai¹; X. Bao¹; C. S. Chow¹; J. Gao²; G. Berden²; J. Oomens²; ¹Wayne State University, Detroit, MI; ²FELIX Facility, Radboud University, Nijmegen, The Netherlands
- TP 574 **Monitoring the Fe(II) Driven Reduction of AMP with Triple Quadrupole Mass Spectrometry**; Jacqueline N Howard¹; Molly T Soper-Hopper¹; Jessica C Bowman¹; Ramanarayanan Krishnamurthy²; Loren Dean Williams¹; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta, USA; ²The Scripps Research Institute, La Jolla, CA
- TP 575 **RNA-small Molecule Complexes as Models for Salt Bridge and Hydrogen Bond Interactions**; Jovana Vusurovic¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Austria
- TP 576 **Comparative Analysis of the Fragmentation of Modified and Unmodified Oligonucleotides**; Ning Li^{1,2}; Babak Basiri¹; Michael G Bartlett¹; ¹University of Georgia, Chemistry Department Athens, GA; ²Shenyang Pharmaceutical University, Shenyang, Liaoning
- TP 577 **Mapping Eukaryotic mRNA-binding Regions on Proteins using High Resolution Mass Spectrometry**; Meeli Mullari¹; Nielsen Lund Michael¹; ¹Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- TP 578 **Förster Resonance Energy Transfer (FRET) Measurements to Probe the Conformation of Gaseous Oligonucleotide Duplexes in the Gas Phase**; Stephen Sciuto¹; Rebecca A Jockusch²; ¹The University of Toronto, Toronto, ON; ²University of Toronto, Toronto, Ontario (ON)
- TP 579 **Mass Spectrometry-based Determination of the Complete Chemical Structure of Saccharomyces Cerevisiae Ribosomal RNAs**; Masato Taoka¹; Yuko Nobe¹; Yuka Yamaki¹; Hideaki Ishikawa²; Yoshio Yamauchi¹; Nobuhiro Takahashi²; Hiroshi Nakayama³; Toshiaki Isobe¹; ¹Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; ²Tokyo University of Agriculture and Technology, Tokyo, Japan; ³RIKEN, Wako, Japan
- TP 580 **Developing Novel Integrated LC-MS Workflows for Oligonucleotide Characterization, High Throughput Mass Confirmation and Impurity Profiling**; HENRY SHION¹; Robert Birdsall¹; Joe Fredette¹; Ying-Qing Yu¹; ¹Waters Corporation, Milford, MA
- TP 581 **On-Line Monitoring of Oligonucleotide Manufacturing Using a Compact Mass Spectrometer**; Stilianos G. Roussis¹; Andrew Rodriguez²; Isaiah Cedillo²; Josh Brooks²; Claus Rentel²; ¹Ionis Pharmaceuticals, Inc., Carlsbad, CA; ²Ionis Pharmaceuticals, Carlsbad, CA
- TP 582 **Use of Tricationic Ion-Pairing Compounds for the Detection of Nucleotides from Single Cells**; ye guan¹; Rachel Vowcicefski¹; Wei Rao¹; Ning Pan¹; Anthony Burgett¹; Zhibo yang¹; ¹University of Oklahoma, department of Chemistry & Biochemistry, Norman, OK
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- TP 583 **Ultra-sensitive Motif-targeting Approach for Measurement of Tyrosine Phosphorylation Stoichiometry in EGFR**; Yen-Chen Liao^{1,2}; Chia-Feng Tsai³; Miao-Hsia Lin¹; Pei-Yi Lin¹; Yasushi Ishihama³; Yu-Ju Chen^{1,2}; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C.); ²Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C.); ³Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan
- TP 584 **Subphosphoproteome Analysis Strategy to Identify Low-abundance Protein Phosphorylation**; Mingliang Ye¹; Mingming Dong¹; Yangyang Bian¹; Lei Li²; Li S.-C. Shawn²; Hanfa Zou¹; ¹Dalian Institute Chemical Physics, CAS Dalian, China; ²Western University, London, Canada
- TP 585 **Comprehensive Phosphoproteome Analysis Reveals Acetylation-engaged Enhancement of Thermogenesis in White Adipocytes**; Hsin-Yi Chang¹; Kosaku Shinoda²; Shingo Kajimura²; Yasushi Ishihama¹; ¹Department of Molecular and Cellular Bioanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ²UCSF Diabetes Center and Department of Cell and Tissue Biology, University of California, San Francisco, CA USA
- TP 586 **Identification of Complex Glycosylated and Disulfide-Bonded Peptides Presented by the MHC Class II Processing Pathway in Melanoma**; Stacy Malaker¹; Michael J Ferracane²; Florence R Depontieu³; Angela L Zarleng¹; Jeffrey Shabanowitz¹; Dina Bai¹; Engelhard H Victor¹; Suzanne L Topalian³; Donald F Hunt¹; ¹University of Virginia, Charlottesville, VA; ²University of Florida, Gainesville, Florida; ³Johns Hopkins University School of Medicine, Baltimore, MD
- TP 587 **Development of Rapid LC-MS3 Methodology for In-depth Structural Analysis of Lewis Antigens and Their Sialylated Derivative Isomers using Authentic Standards**; Yaping Lin¹; Chein-Hung Chen²; Fang-Chi Liu²; Chia-Lin Wu²; Jung-Lee Lin²; Chien-Tai Ren²; Chung-Yi Wu²; Chung-Hsuan Chen²; ¹Academia sinica, Taipei, Taiwan; ²Academia Sinica, Taipei, Taiwan
- TP 588 **Sialo-glycoproteomic Profiling using Zwitter-Ionic Hydrophilic Interaction Chromatography (ZIC-cHILIC)**; Yu-Hsien Lin¹; Yi-Ju Chen¹; Yu-Ju Chen¹; ¹Academia Sinica, Taipei, Taiwan
- TP 589 **Proteome Dynamics Reveal Temporal Regulation of O-GlcNAcylation/phosphorylation in Determining Apoptosis of Activated B Cells**; Hsin-Yi Wu¹; Jung-Lin Wu^{2,3}; Cheng-Tsung Lu⁴; Yi-Ju Chen⁵; Tzong-Yi Lee⁴; Chih-Wei Chien⁵; Yi-Ting Wang⁵; Chun-Cheng Lin⁶; Kay-Hooi Khoo⁷; Yu-Ju Chen⁵; Kuo-I Lin²; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ²Genomics Research Center, Academia Sinica, Taipei, Taiwan; ³Institute and Department of Microbiology and Immunology, National Yang-Ming University, Taipei, Taiwan; ⁴Department of Computer Science and Engineering, Yuan Ze University, Taipei, Taiwan; ⁵Institute of Chemistry, Academia Sinica, Taipei, TAIWAN (R.O.C.); ⁶Department of Chemistry, National Tsing Hua University, Taipei, Taiwan; ⁷Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan



- TP 590 **Efficient Enrichment of SUMOylated Peptides from Alpha-lytic Protease Digest Using K-ε -GG Remnant Immuno-affinity Purification;** Hongbo Gu¹; Xiaoying Jia¹; Jian Min Ren¹; Elizabeth Komives²; Matthew P Stokes¹; ¹Cell Signaling Technology, Danvers, MA; ²Department of Chemistry and Biochemistry, UCSD, La Jolla, CA
- TP 591 **An Improved Strategy for In-depth and Site-specific Analysis of the SUMO Proteome;** Ivo A. Hendriks¹; Clifford Young¹; Michael L. Nielsen¹; ¹NNF Center for Protein Research, Copenhagen, Denmark
- TP 592 **Ubiquitinated Proteins in MDSC Exosomes Analyzed by High Resolution Tandem Mass Spectrometry;** Katherine Adams¹; Yan Wang¹; Suzanne Ostrand-Rosenberg²; Catherine Fenselau¹; ¹University of Maryland, College Park, MD; ²University of Maryland, Baltimore County Baltimore, MD
- TP 593 **Low Mass Ions in Peptide CID Spectra are Diagnostic of Lysine Posttranslational Modifications;** Tobias Maile¹; Tommy K Cheung¹; Corey Bakalarski¹; Marie Classon¹; David Amott¹; ¹Genentech Inc, South San Francisco, CA
- TP 594 **Quantitative Profiling of the Enzymatic Activity of the Protein Lysine Mono-methyltransferase SMYD2 using SILAC-based Proteomics;** Jonathan B Olsen¹; Xing-Jun CAO²; Bomie Han¹; Lisa Hong Chen¹; Alexander Horvath¹; Timothy I Richardson¹; Robert M Campbell¹; Benjamin A Garcia²; Hannah Nguyen¹; ¹Eli Lilly and Company, Indianapolis, IN; ²University of Pennsylvania, Philadelphia, PA
- TP 595 **Characterizing Post-Translationally Modified Peptides by High-Resolution FAIMS Coupled to Electron Transfer Dissociation;** Matthew Baird¹; Alexandre A Shvartsburg¹; ¹Wichita State University, Wichita, KS
- TP 596 **Innovative Characterization of Hair from pre-Hispanic Andean Mummies using Mass Spectrometry;** Margaux Fresnais¹; Pascale Richardin²; Marcela Sepúlveda³; Emmanuelle Leize-Wagner¹; Armelle Charrié-Duhaut¹; ¹Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), UMR 7140 CNRS-Université de Strasbourg, Strasbourg, France; ²Centre de Recherche et de Restauration des Musées de France (C2RMF), Paris, France; ³Laboratorio de Análisis e Investigación Arqueométricas, Instituto de Alta Investigación, University of Tarapacá, Arica, Chile
- TP 597 **Identification and Characterization of Covalent Modification of Catechol Estrogens on Proteins ;** Huei-Chen Liang¹; Chieh-Ming Fang¹; Ming-Chun Ku¹; Shu-Hui Chen¹; ¹Chemistry Dept. NCKU, Tainan, Taiwan (R.O.C.)
- TP 598 **Comprehensive Analysis of Post-translational Modifications in Proteins Exposed to Metal Catalyzed Oxidation;** Martin Rykær¹; Birte Svensson²; Kim Henriksen³; Per Hågglund²; ¹Technical University of Denmark, Kgs Lyngby, Kgs Lyngby; ²Technical University of Denmark, Systems biology, KGS Lyngby., DK; ³Nordic Bioscience A/S, Herlev, DK
- TP 599 **Quantitative Profiling of Prokaryotic Post Translational Modifications;** Charles L Farnsworth¹; Jian Min Ren²; Jake A Namaroff²; Xiaoying Jia¹; Kimberly A Lee²; Matthew P Stokes²; ¹Cell Signaling Technology, Danvers, MA; ²Cell Signaling Technology, Inc. Danvers, MA
- TP 600 **Charged Isotope Tag Improves Identification of Hydrophobic Peptide-Ligand Adducts;** Melissa Budelier¹; James Janetka¹; Douglas Covey¹; Alex Evers¹; ¹Washington University in St. Louis, St. Louis, MO
- TP 601 **Alkylamine Ion-pairing Agents for Improved Positive Mode Electrospray Ionization Analysis of Sulfated Peptides;** Phillip McClory¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI
- TP 602 **N-Terminal Charged-based Fractional Diagonal Chromatography (ChaFRADIC) to Study Proteolytic Events in Procoagulant Platelets;** Fiorella Andrea Solari¹; Saskia A. Venne²; Nadine J.A. Mattheij³; Julia M. Burkhart²; Frauke Swieringa³; Peter W. Collins⁴; Judith M.E.M. Cosemans³; Albert Sickmann²; Johan W.M. Heemskerk³; René P Zahedi²; ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; ²Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany; ³Department of Biochemistry, Cardiovascular Research Institute Maastricht (CARIM) Maastricht University Maastricht, Maastricht, Netherlands; ⁴Arthur Bloom Haemophilia Centre, School of Medicine, Cardiff University, Cardiff, United Kingdom
- TP 603 **Utilizing TIMS Mass Spectrometry to Resolve Competitive Isomeric Post-Translational Modifications;** Joshua Silveira¹; Joe Gomez²; Melvin Park¹; Kristofer Fritz³; ¹Brucker Daltonics, Billerica, MA; ²University of Colorado, Anschutz Medical Campus, Aurora, CO; ³University of Colorado, Anschutz Medical Campus, Denver, CO
- TP 604 **System-wide Analysis of the Human Arginine Methylome;** Sara C. Larsen¹; Kathrine B. Sylvestersen¹; Andreas Mund¹; Maria V. Madsen¹; David Lyon¹; Jeremy A. Daniel¹; Lars J. Jensen¹; Michael L. Nielsen¹; ¹NNF Center for Protein Research, Copenhagen, DENMARK
- TP 605 **Method Development for Complete Mutation and Posttranscriptional Modification Characterization of KRAS4b using Recombinant Proteins in Combination with LC-MS/MS;** Zhaojing Meng¹; William Gillette¹; Stephen Andrew¹; Ming Zhou¹; ¹Frederick National Laboratory for Cancer Research, Frederick, MD

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- TP 606 **Multiplexed Targeted Analysis of Post-translational Modifications: Robust and Reproducible Quantitation using isobaric Labels and MS3 Analysis;** Brian Erickson¹; Robert A Everley¹; Christopher M Rose¹; Alison R Erickson¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA
- TP 607 **Comparative Phosphoproteomic Analysis of Hippocampal Tissue in a Non-Human Primate Model of Type 1 Diabetes Maintained with Exogenous Insulin;** Fang-Ke Huang¹; Jose Morales-Corraliza^{2,3}; Paul M. Mathews^{2,3}; Thomas A. Neubert¹; ¹Skirball Institute of Biomolecular Medicine, New York University School of Medicine, New York City, NY; ²Center for Dementia Research, Nathan Kline Institute, Orangeburg, NY; ³Department of Psychiatry, New York University Langone Medical Center, New York City, NY
- TP 608 **Large-scale Targeted Analysis of Post-translational Modifications by Internal Standard-Triggered Parallel Reaction Monitoring: Application to Determination of Phosphorylation Site Occupancy;** Bruno Doman¹; Sara Rosati¹; Adele Bourmaud¹; Sebastien Gallien¹; ¹Luxembourg Clinical Proteomics Center, Strassen, Luxembourg
- TP 609 **Global Phosphoproteomics of Targeted Combinatorial Therapy in Hepatocellular Carcinoma to Identify Molecular Signatures of Effective Therapy;** Joseph Capri¹; Whitaker Cohn¹; Thuc Le¹; Kym F Faul¹; Julian P Whitelegge¹; ¹UCLA, Los Angeles, CA
- TP 610 **Quantitative Analysis of the Cdk-dependent Phosphoproteome in S. Pombe using SILAC and Tandem Mass Tags;** Andrew W Jones^{1,2}; Matthew Swaffer²; Jenny T.C Ho³; Helen Flynn¹; Paul Nurse²; Gary Woffendin³; Madalina Oppermann³; Ambrosius P Snijders¹; ¹Proteomics Technology Platform, The Francis Crick Institute, London, UK; ²Cell Cycle Laboratory, The Francis Crick Institute, London, UK; ³Thermo Fisher Scientific, Hemel Hempstead, Hemel Hempstead, UK

- TP 611 **Phosphoproteome Analysis Reveals Rapid Reprogramming of Signaling Networks of Drug Treated Cancer Cells;** Heiner Koch^{1,2,3}; Melanie Schoof¹; Benjamin Ruprecht¹; Susan Klaeger¹; Scarlet Beck⁴; Martin Frejno^{1,5}; Mathias Wilhelm¹; Hannes Hahne⁶; Bernhard Kuster^{1,2,3,7}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²German Cancer Consortium (DKTK), Muenchen, Germany; ³German Cancer Research Center, Heidelberg, Germany; ⁴Max Planck Institute for Biochemistry, Martinsried, Germany; ⁵Oxford University, Oxford, United Kingdom; ⁶OmicScouts GmbH, Freising, Germany; ⁷Center for Integrated Protein Science, Munich, Germany
- TP 612 **Effect of Exercise on Skeletal Muscle Phosphoproteome in Obese Insulin Resistant Adults;** DanJun Ma¹; Lisa Guth²; Yue Qi¹; Michael Caruso¹; Xiangmin Zhang¹; Jeffrey Horowitz²; Zhengping Yi¹; ¹Wayne State University, Detroit, MI; ²University of Michigan, Ann Arbor, MI
- TP 613 **Quantitative Phosphoproteomic Analysis of Circadian Cycling in Genetically Modified Arabidopsis;** Jae Choi¹; Jenny Chen²; John D Rogers¹; Dmitri A Nusinow³; Bradley S Evans³; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA; ³Donald Danforth Plant Science Center, St Louis, MO
- TP 614 **Differential Mass Spectrometry Analysis Reveals Differential Hypoxic Response in Ovarian Cancer Cells with Different Metastatic Potential;** Xuemei Zeng¹; Huang Huang¹; Xin Huang¹; Nathan A Yates¹; ¹University of Pittsburgh, Pittsburgh, PA
- TP 615 **Rapid Quantitative Phosphoproteome by Tandem Mass Tags;** Haiyan Tan¹; Bing Bai²; Xusheng Wang²; Yuxin Li²; Ji-Hoon Cho²; Tim Shaw²; Junmin Peng²; ¹St.Jude Children's Research Hospital, Memphis, TN; ²St Jude Children's Research Hospital, Memphis, TN
- TP 616 **High Throughput Multiplexed Phosphoproteomics Identifies Drivers of Resistance to ALK Inhibitor Treatment in Lung Cancer;** Amanda L. Edwards^{1,2}; Luc Friboulet^{1,2}; Rosa Frias^{1,2}; Kristine Yu³; David Ruddy³; Jeffrey A. Engelman^{1,2}; Wilhelm Haas^{1,2}; ¹Massachusetts General Hospital Cancer Center, Charlestown, MA; ²Harvard Medical School, Boston, MA; ³Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA
- TP 617 **Inferring Kinase Network Activity from Activation-loop Phosphopeptides by Data-Independent Acquisition MS;** Sander Piersma¹; Richard R de Haas¹; Jaco C Knol¹; Thang V Pham¹; Henk MW Verheul¹; Connie R Jimenez¹; ¹VU University medical center, Amsterdam, The Netherlands
- TP 618 **Prediction of Protein Kinase Substrates using Primary Sequence Preference and Quantitative Phosphoproteomics;** Haruna Imamura¹; Pasrawin Taechawattananant¹; Omar Wagih²; Naoyuki Sugiyama¹; Pedro Beltrao²; Yasushi Ishihama¹; ¹Kyoto University, Kyoto, Japan; ²European Bioinformatics Institute, European Molecular Biology Laboratory, Hinxton, Cambridge, United Kingdom
- TP 619 **Absolute Quantitation of Site-specific Phosphorylation of Insulin Receptor by A Nano UPLC-MS Method;** Zhongping Liao¹; Kyoung-soo Choi¹; Jason X Tang¹; ¹Eli Lilly and Company, Indianapolis, IN
- TP 620 **Evaluation of Search Engines for Phosphopeptide Identification and Quantitation;** Xiaoyue Jiang¹; David M Horn¹; Ryan D Bomgarden²; Tara Schroeder³; Rosa I Viner¹; Andreas Huhmer¹; Steven Danielson⁴; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Rockford, IL; ³Thermo Fisher Scientific, Somerset, NJ; ⁴Thermo Fisher, San Jose, CA
- TP 621 **Dimethylated Alanine (DiAla)-assisted Large-scale Protein Phosphorylation Stoichiometry Characterization;** Qing Yu¹; Yu Feng²; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, Wisconsin; ²University of Wisconsin-Madison, Madison, WI
- TP 622 **High Resolution-Enabled 12-plex DiLeu Tagging for Quantitative Phosphoproteomics Profiling of Vascular Smooth Muscle Cells;** Xiaofang Zhong¹; Christopher Lietz¹; Xudong Shi¹; Amanda Buchberger¹; Dustin Frost¹; Craig Kent¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- TP 623 **Sensitive and Accurate Quantitation of Phosphopeptides using TMT Isobaric Labeling Technique;** Xiaoyue Jiang¹; Ryan D Bomgarden²; Rosa I Viner¹; Andreas Huhmer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Rockford, IL

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- TP 624 **Using Native MS to inform Statistical Thermodynamic Models of Cooperativity;** Melody Pepsi Holmquist¹; Elihu C Ihms¹; Vicki H Wysocki¹; Mark P Foster¹; ¹Ohio State University, Columbus, OH
- TP 625 **Native MS analysis of chemically stabilized protein complexes: evidence for non-covalent stabilization of protein-protein interactions;** Roman Subbotin¹; Dominic Paul B Olinares¹; Julio C Padovan¹; Megan Kelley¹; Zheng Ser¹; Brian T Chait¹; ¹The Rockefeller University, New York, NY
- TP 626 **Probing Nucleotide-dependent Changes in the Oligomeric State of MORC Proteins using Native Mass Spectrometry;** Jonathan Johnston¹; Linda Yen²; Steven E Jacobsen²; Alma L Burlingame¹; ¹UCSF, San Francisco, CA; ²UCLA, Los Angeles, CA
- TP 627 **Characterization of a Protein-DNA Complex by Native Mass Spectrometry and Ultraviolet Photodissociation;** Jake Rosenberg¹; Alyssa Garabedian²; Fenfei Leng²; Francisco Fernandez-Lima²; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Florida International University, Miami, FL
- TP 628 **Investigating the Gas-Phase Conformation of Fibroblast Growth Factor 1 upon Binding of Heparin/HS Using Traveling Wave Ion Mobility Spectrometry (TWIMS);** Yuejie Zhao¹; Jon Amster¹; Arunima Singh²; Robert Woods²; Yongmei Xu³; Jian Liu³; Chengli Zong²; Geert-Jan Boons²; Fuming Zhang⁴; Robert Linhardt⁴; ¹University of Georgia, Chemistry Department Athens, GA; ²University of Georgia, CCRC Athens, GA; ³University of North Carolina, Chapel Hill, NC; ⁴Rensselaer Polytechnic University, Troy, NY
- TP 629 **Screening Glycolipids Against Proteins in vitro using Picodiscs and Electrospray Ionization Mass Spectrometry;** Jun Li¹; Xuxin Fan¹; Elena N Kitova¹; John S Klassen¹; ¹University of Alberta, Edmonton, AB, Canada
- TP 630 **Detecting Protein-Glycolipid Interactions using Glycomicelles and CaR-ESI-MS;** Ling Han¹; Elena N Kitova¹; John S Klassen¹; ¹University of Alberta, Edmonton, Canada
- TP 631 **Characterization of Heparin Interactions with its Client Proteins: Mapping Minimal Protein-Binding Domains within Glycosaminoglycan Chains using Top-down mass spectrometry;** Yunlong Zhao¹; Igor A Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA
- TP 632 **Screening Human Milk Oligosaccharides Against Proteins using Catch-and-Release Electrospray Ionization Mass Spectrometry;** Yajie Chen¹; Km Shams-Ud-Doha¹; Elena N Kitova¹; Lars Bode²; John S Klassen¹; ¹University of Alberta, Edmonton, Canada; ²University of California, San Diego La Jolla, CA

- TP 633 **Label Free, LC-MS Based Approaches to Quantitate Small Molecule-Receptor Binding;** Xun Chen; Merck Research Labs, Kenilworth, NJ
- TP 634 **Label-free Size Exclusion Chromatography Mass Spectrometry for the Characterization of Protein Complex Composition and Stability;** Paola Cavaliere¹; Nadia Iqbal¹; Noah E. Dephoure¹; ¹Weill Cornell Medical College, New York, NY
- TP 635 **Information-Rich Gas-Phase Analysis of Non-Covalent Protein Complexes and Released Subunits for Primary and Quaternary Structure Analysis;** Deepali Rathore¹; Forouzan Aboufazel¹; Eric D. Dodds¹; ¹University of Nebraska-Lincoln, Lincoln, NE
- TP 636 **Study of Noncovalent Interactions of Hydroxylated Polybrominated Diphenyl Ethers with Serum Albumins and Estrogen Receptors Using Ion Mobility Spectrometry-Mass Spectrometry;** Qiang Ma¹; Liang-Hong Guo²; ¹Chinese Academy of Inspection and Quarantine, Beijing, CHINA; ²Chinese Academy of Sciences, Beijing, CHINA
- TP 637 **Investigating The Noncovalent Complex Formation of Proteins with Electrolytic Ligands in Gas Phase;** Mehmet Atakay¹; Haci Mehmet Kayili^{1,2}; Bekir Salih¹; ¹Hacettepe University, Department of Chemistry, Ankara, Turkey; ²Çankırı Karatekin University, Çankırı, Turkey
- TP 638 **Probing the Stability of Noncovalent Interactions Responsible for Covalently Linked Diubiquitin Ion Structure using nESI-TWIMS-MS and CIU;** Nicole Wagner¹; David H Russell¹; ¹Texas A&M University, College Station, TX
- TP 639 **Identification of Grp78/BiP Protein Complexes using Affinity Mass Spectrometry;** Dapeng Chen¹; Yan Wang¹; Eva R. Chin¹; ¹University of Maryland, College Park, MD
- TP 640 **Comparison of Affinity-Purification Mass Spectrometry Workflow for Characterisation of Protein Complexes;** Lu Yu¹; Mercedes Pardo²; Jyoti Choudhary²; ¹Wellcome Trust Sanger Institute, Hinxton, Cambridgeshire; ²Wellcome Trust Sanger Institute, Cambridge, United Kingdom
- TP 641 **Application of Affinity-purification Mass Spectrometry Based Predictive Mapping for Identification of RBM45 Protein Interactors in Amyotrophic Lateral Sclerosis;** Krystine Garcia¹; Yang Li²; Mahlon Collins^{2,3}; Jiyan An²; Rachel Geiser²; Tony Tegeler¹; Kristine Tsantilas¹; Robert Bowser^{2,3}; Patrick Pirrotte¹; ¹TGen, Phoenix, AZ; ²St. Joseph's Hospital and Medical Center, Phoenix, AZ; ³University of Pittsburgh School of Medicine, Pitts, PA
- TP 642 **Nanoprobe-based Affinity Mass Spectrometry for Identification of Binding Glycotopes and Protein-Protein Interaction of Galectin-8;** Pin-Rui Su¹; Chen Yi-Ju²; Lin Yu-Hsien³; Chen Yu-Ju²; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ³Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan
- TP 643 **Site-specific Characterization of Binding Interfaces in Gaseous HIV-1 RNA-protein Complexes;** Eva-Maria Schneeberger¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Austria
- TP 644 **Novel Blue-Native-PAGE and Targeted Mass Spectrometry Strategy Enable robust and Accurate Quantification of the Kinetics of Protein-Ligand Interactions in Plasma;** Shichen Shen¹; Xiaotao Duan²; Bo An¹; Yang Qu¹; Joseph Balthasar¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Beijing Proteome Research Center, Beijing, China
- TP 645 **A New Carbene Probe for Efficient Protein Footprinting Allows Mapping of Binding Sites by Mass Spectrometry;** Lucio Manzi¹; Andrew Barrow¹; Daniel Scott¹; Robert Layfield¹; Timothy Wright¹; John Moses¹; Neil Oldham¹; ¹University of Nottingham, Nottingham, UK
- TP 646 **Charting the Temporal Landscape of EGF-stimulated EGFR Proteome** ; Yue Chen¹; Sung Yun Jung¹; Mei Leng¹; Jong Min Choi¹; Antrix Jain¹; Anna Malovannaya¹; Yi Wang¹; Jun Qin¹; ¹Baylor College of Medicine, Houston, TX
- TP 647 **Development of a Novel Bioanalytical Platform for Anti-Drug Antibody using Immunocapture-LC/MS;** Lin-Zhi Chen¹; David Roos²; Elsy Philip²; ¹Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; ²Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT
- TP 648 **Novel Regulators of Alternative NF-κB Pathway Identified through Chemical Proteomics;** Bekim Bajrami¹; Michelle Ols¹; John Anderson¹; Benbo Gao¹; Brian Lucas¹; Erik Hett¹; Alan Buckler¹; Peter Juhasz¹; Ru Wei¹; ¹Biogen Inc., Cambridge, MA
- TP 649 **Proteomic Analysis Provides Clues about Normal FUS Function and Its Role in ALS;** Jing Chen¹; Marisa Kamelgarn¹; Alexandra Arenas¹; Jianjun Zhai¹; Haining Zhu¹; Jozsef Gal¹; ¹University of Kentucky, Lexington, KY
- TP 650 **Global Analyses of the Oligomerization, Composition, and Dynamics of Membrane-Associated Protein Complexes;** Zach McBride¹; Aryal Uma¹; Chen Donglai¹; Jun Xie¹; Daniel Szymanski¹; ¹Purdue University, West Lafayette, IN
- TP 651 **Mass Spectrometry Cleavable Cross-linking Approach for Large-scale Identification of Protein-Protein Interactions;** Jayanta Kishor Chakrabarty¹; Apeksha Bhatt¹; Saiful M Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- TP 652 **Relative Abundance Comparative Analysis of ROS-induced Poly(ADP-ribose)-Associated Proteins by LC-MS/MS and Spectral Counting;** Argel Islas-Robles^{1,2}; Frances M Munoz³; Serrine S Lau²; Terrence J Monks²; ¹University of Arizona, Tucson, AZ; ²Wayne State University, Detroit, MI; ³Drexel University, Philadelphia, PA
- TP 653 **Fourier Transform Algorithm for Analysis of Mass Spectra for Heterogeneous Ions with Repeated Subunits;** Sean P Cleary¹; Jesse W Wilson¹; Avery M Thompson¹; James Prell¹; ¹University of Oregon, Eugene, OR
- TP 654 **Development of Mass Spectrometry Method for the Unbiased Detection of Cytomegalovirus Proteins in Human Brain Tumor Specimens;** Dhiman Ghosh¹; Brian P Milless²; Philip R Gafken³; Charles S Cobbs¹; ¹Swedish Neuroscience Institute, Seattle, Washington; ²Fred Hutchinson Cancer Research Center, Seattle, Washington; ³Fred Hutchinson Cancer Research Center, Seattle, WA
- TP 655 **Edgotypes and Quantitative Mass Spectrometry;** James Bruce¹; Juan Chavez¹; Jimmy K Eng¹; Arti Navare¹; Devin Schweppe¹; Xia Wu¹; Xuefei Zhong¹; ¹University of Washington, Seattle, WA
- TP 656 **Histidine, Arginine's Versatile Cousin;** Amina S Woods¹; Ludovic Muller¹; Aurelie Roux²; Damon Barbacci³; Shelley N Jackson¹; ¹NIH/NIDA-IRP, Baltimore, MD; ²All Children's Hospital Johns Hopkins Medicine, Saint Petersburg, FL; ³Ionwerks Inc, Houston, TX
- TP 657 **Examination of Aptamer-Protein Complex Structure by Mass Spectrometry;** Guo-Ming Hung¹; Pang-Hung Hsu¹; ¹Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan
- TP 658 **Cross-linked PSMs in pepXML: a Common Format for Storing Cross-linked Search Results;** Michael R. Hoopmann¹; Luis Mendoza¹; Eric W. Deutsch¹; David Shteynberg¹; Robert L Moritz¹; ¹Institute for Systems Biology, Seattle, WA
- TP 659 **The Analysis and Identification of STAT3 Interactions and Modifications in the Mitochondria of Cancer Cells;** Daniel Garama¹; Ching-Seng Ang²; Nick Williamson²; Daniel Gough¹; ¹Hudson Institute of Medical Research, Melbourne, Australia; ²Bio 21 Institute, Melbourne, Australia

PROTEOMICS: CLINICAL APPLICATIONS (DEVELOPMENT TOWARD CLINICAL APPLICATION)
660 - 681

- TP 660 **Proteomic Profiling of Human Islets Collected from Pancreatic Tissue Sections using Laser Capture Microdissection;** Lina Zhang¹; Giacomo Lanzoni²; Matteo Battarra²; Luca Inverardi²; Qibin Zhang³; ¹, Kannapolis, NC; ²Diabetes Research Institute, University of Miami, Miami, FL; ³Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC
- TP 661 **Using Quantitative Proteomics to Profile Changes in Individual Immune Cell Types during an Immune Response;** Allison Galassie¹; Johannes Goll²; Parimal Samir³; Travis Jensen²; Kristen L Hoek⁴; Leigh M Howard⁵; Tara M Allos⁴; Xinnan Niu⁴; Sebastian Joyce^{4,6}; Kathryn M Edwards⁵; Andrew J Link⁴; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²The EMMES Corporation, Rockville, MD; ³Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; ⁴Department of Pathology, Microbiology, and Immunology, Vanderbilt University School of Medicine, Nashville, TN; ⁵Vanderbilt Vaccine Research Program; Division of Infectious Diseases, Department of Pediatrics, Vanderbilt University School of Medicine, Nashville, TN; ⁶Veterans Administration Tennessee Valley Healthcare System, Nashville, TN
- TP 662 **LC-MRM Quantification of Protein Biomarkers in Human Saliva: In Saliva Veritas?** Jerome Vialaret¹; Nora Nowak¹; Audrey Gabelle²; Sylvain LEHMANN¹; Christophe Hirtz¹; ¹LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; ²Centre Memoire Ressources Recherche Languedoc-Roussillon, CHU Montpellier, Montpellier, France
- TP 663 **Elucidating Cellular Heterogeneity in Tumors: a Combination of Antibody-Based Cellular Pre-Fractionation and Ultrasensitive Proteomics;** Evelynne Maes¹; Nathalie Cools²; Inge Mertens^{1,3}; Dirk Valkenborg^{1,3,4}; Patrick Pauwels⁵; Geert Baggerman^{1,6}; ¹VITO, Mol, Belgium; ²Laboratory of Experimental Hematology, Vaccine & Infectious Disease Institute (VAXINFECTIO), University of Antwerp, Antwerp, Belgium; ³Center for Proteomics, Antwerp, Belgium; ⁴Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Diepenbeek, Belgium; ⁵Pathology Department, University Hospital Antwerp (UZA), Antwerp, Belgium; ⁶Center for Proteomics, Antwerp, Belgium
- TP 664 **LC-MS Platform for Identifying Protein Targets of Small-Molecule Binding Relevant to Disease and Metabolism;** Reid O'Brien Johnson¹; Brett Lomenick¹; Jing Huang¹; Joseph A Loo¹; ¹UCLA, Los Angeles, CA
- TP 665 **Simple, Robust, Highly Productive Methodology for LC-MS/MS Quantitative Analysis of Laser Capture Microdissected Tissue from FFPE Biopsies Requiring 10,000 Cells;** John P Shapiro¹; Hannah Komar¹; Phil Gaffen²; Philip Hart¹; Darwin Conwell¹; Gregory Lesinski¹; ¹Ohio State University, Columbus, Ohio; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- TP 666 **Quantifying Signalling Pathway Activity using iMALDI (Immuno-MALDI);** Robert Popp¹; Andrew G Chambers¹; Adriana Aguilar-Mahecha²; Oliver Pötz³; Mark Basik²; Christoph H. Borchers^{4,5,6}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Department of Oncology, McGill University, Montreal, QC, Canada; ³Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; ⁴University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁶Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada
- TP 667 **Automation of an immuno-MALDI assay for Quantifying Signalling Pathway Activity;** Robert Popp¹; Björn Fröhlich¹; Andrew G Chambers¹; Yassene Mohammed¹; ²Adriana Aguilar-Mahecha³; Oliver Pötz⁴; Mark Basik³; Christoph H. Borchers^{1,5,6}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; ³Department of Oncology, McGill University, Montreal, QC, Canada; ⁴Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁶Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada
- TP 668 **Can volumetric Absorptive Micro Sampling in the Presence of a Stable-Isotope Labeled Protein Standard Control Pre-Analytical Variability in Proteomics?** Irene van den Broek¹; Qin Fu¹; Kevin Millis²; Timothy Eckersley²; William W Wood²; Michael P Kowalski³; Tara R Jones-Roe³; Stuart Kushon⁴; Bobby Virasingh⁴; Jennifer E Van Eyk¹; ¹Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; ²Cambridge Isotope Laboratories, Inc. Tewksbury, MA; ³Beckman Coulter Life Sciences, Indianapolis, IN; ⁴Neoteryx, Torrance, CA
- TP 669 **Methodological Advances Applied to a Biomarker Study of Complex Samples from a Diseased Clinical Cohort of Limited Sample Availability;** Stephen Kostel¹; Patricia Cho¹; Hui Zhou¹; John Froehlich¹; Richard Lee¹; ¹Boston Children's Hospital, Harvard Medical School Boston, MA
- TP 670 **Combined Analysis of Nucleic Acids and Protein for Cancer Research;** Jared Isaac¹; Mazi Mohiuddin²; ¹Thermo Fisher Scientific, Kalamazoo, MI; ²Thermo Fisher Scientific, San Jose, CA
- TP 671 **Human Plasma Proteome Analysis using Meter-Long Monolithic Silica Columns with Match-between-Runs;** Yi Ting Wang¹; Chia-Feng Tsai²; Kazuhiro Sonomura^{1,3}; Yasushi Ishihama²; Fumihiko Matsuda¹; ¹Center for Genomic Medicine, Graduate School of Medicine Kyoto University, Kyoto, Japan; ²Graduate School of Pharmaceutical Sciences Kyoto University, Kyoto, Japan; ³Life Science Research Center, Technology Research Laboratory, Shimadzu Corporation, Kyoto, Japan
- TP 672 **A Chromosome-Centric Protein-Protein Interaction Profiling of MS-Based Proteome Datasets Derived from Laser-Microdissected Cancerous Cells of Lung Cancer Subtypes;** Kiyonaga Fujii¹; Hiroyuki Kimura¹; Hideki Marushima¹; Rie Tagaya¹; Hisashi Saji¹; Noriaki Kurimoto¹; Sayaka Mikami²; Yasuhiko Bando²; Noboru Nakayama¹; ²Harubumi Kato³; Toshihide Nishimura^{1,2}; Haruhiko Nakamura¹; ¹St. Marianna University School of Medicine, Meguro-ku, Tokyo; ²Biosys Technologies, Inc., Tokyo, Japan; ³Niizashi Central General Hospital, Saitama, Japan
- TP 673 **High-resolution Quantitative Metaproteomics Pipeline: Documenting Effects of Dietary Changes;** Boris Zybailov¹; Stephanie Byrum¹; Galina Glazko¹; Lisa Orr¹; Dorothy Kieffer²; Sean Adams¹; Samuel Mackintosh¹; John Arthur¹; Brian D. Piccolo¹; Nosratola D. Vaziri³; Shuman Liu³; Wei L. Lau³; Mahyar Khazaeli³; Mary E. Moore⁴; Roy J. Martin⁵; ¹University of Arkansas for Medical Sciences, Little Rock, AR; ²University of California, Davis, Davis, CA; ³Division of Nephrology, University of California, Irvine, Irvine, CA; ⁴Dept. of Food Science and Technology, University of California, Davis, Davis, CA; ⁵Obesity & Metabolism Research Unit, USDA, Davis, CA
- TP 674 **Investigation of Neutrophilic Proteins/Peptides in Periprosthetic Tissue by MALDI Imaging Mass Spectrometry;** Rémi Longuespée¹; Rita Casadonte¹; Mark



- Kriegsmann²; Mike Otto^{1,3}; Sascha Gravius⁴; Thomas Randau⁴; Soeren-Oliver Deininger⁵; Edwin De Pauw⁶; Jörg Kriegsmann^{1,3}; ¹Proteopath GmbH, Trier, Germany; ²University of Heidelberg, Heidelberg, Germany; ³Center for Histology Cytology and Molecular Diagnostics, Trier, Germany; ⁴University Bonn, Bonn, Germany; ⁵Bruker Daltonik, Bremen, Germany; ⁶University of Liege, GIGA-Proteomics Liege, Belgium
- TP 675 **Generation of High Quality MALDI-TOF Serum Mass Spectra to Detect Hepatocellular Carcinoma in High-Risk Patients;** Nicholas F Dupuis¹; Maximilian Steers¹; Alex A Nickel¹; Gary P Pestano¹; ¹Biodesix, Inc., Boulder, Colorado [CO]
- TP 676 **Correlating Apolipoprotein Proteoform Profiles to Cardiovascular Disease Risk Factors: a Translational Top-Down Proteomics Approach to Pathophysiology;** Henrique dos Santos Seckler¹; Kyunggon Kim¹; Luca Fornelli¹; Paul M Thomas¹; Philip Compton¹; John T Wilkins²; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Northwestern Feinberg School of Medicine, Chicago, IL
- TP 677 **Application of Tissue Surrogate for Variance Calibration in Mass Spectrometry Based Amyloidosis Diagnosis;** Han-Yin Yang¹; Andrew N Hoofnagle¹; Michael J MacCoss¹; ¹University of Washington, Seattle, WA
- TP 678 **Quantitative Analysis of Protein Composition in Amyloid Plaques from FFPE Specimens using Parallel Reaction Monitoring (PRM);** Maria Stella Ritorto¹; Oana Madalina Mereuta¹; Janine Pichardo¹; Ahmet Dogan¹; ¹Memorial Sloan Kettering Cancer Center, New York, NY
- TP 679 **Analysis of Native Proteolytic BNP Variants: Simultaneous Separation of Multiple Samples using Capillary Electrophoresis-Mass Spectrometry with Multi-Segment Injection;** Shenyan Zhang¹; Koen Raedschelders¹; Jennifer Van Eyk¹; ¹Barbra Streisand Women's Heart Center, Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA - California
- TP 680 **Implementation of sKALIP to Identify the Substrates of CDKL5, a Kinase Linked to Severe Neurodevelopmental Disorders;** Justine Arrington¹; Juan Sebastian Paez Paez²; Weiguo Andy Tao¹; ¹Purdue University, West Lafayette, IN; ²National University of Colombia, Bogota, Colombia
- TP 681 **Dried Blood Spots as a Simple Sample Collection Tool for Personalized Medicine;** Jeffrey J. Jones¹; Ryan Benz¹; Phong Cun¹; William Smith¹; John Blume¹; ¹Applied Proteomics Inc., San Diego, CA

PROTEOMICS: INFECTIOUS DISEASES 682 - 702

- TP 682 **Characterization of the Host Proteome within Virion Particles of Sindbis Virus;** Andrew Kilianski¹; Amanda Piper²; Vancini Ricardo²; Raquel Hernandez²; Trevor Glaros¹; ¹ECBC, Apg, MD; ²North Carolina State University, Raleigh, North Carolina
- TP 683 **Mass Spectrometric Analysis of the Human Pathogen *Cryptosporidium parvum*;** John Robert Haserick¹; Deborah R Leon¹; Yi Pu^{1,2}; John Crawford Samuelson¹; ³Catherine E Costello¹; ¹Boston University School of Medicine, Boston, MA; ²Boston University, Boston, MA; ³Boston University School of Dental Medicine, Boston, MA
- TP 684 **The Detection of a Clinically Relevant β -lactamase, CTX-M-15, Using MALDI-TOF MS;** Jonathan B. Thacker¹; Brad S. Pierce¹; Kevin A. Schug¹; ¹University of Texas at Arlington, Arlington, TX
- TP 685 ***Pseudomonas aeruginosa* Develops Ciprofloxacin Resistance from Low to High Level with Distinctive Proteome Changes;** Jianhe Peng¹; Jeffrey Hill²; ¹Experimental Therapeutics Centre, A-STAR, Singapore, Singapore; ²Experimental Therapeutics Centre, A-STAR, Singapore, Singapore
- TP 686 **Proteomics Analysis of *Chlamydia trachomatis*: Virulence-Plasmid Mediated Protein Expression Changes;** Christopher C R Grant¹; Stuart McCorrister¹; Michael Patton²; Harlan Caldwell²; Garrett R Westmacott¹; Grant McClarty¹; ¹National Microbiology Laboratory, Public Health Agency of Canada, Winnipeg, Canada; ²Chlamydial Diseases Section, Laboratory of Clinical Infectious Diseases NIAID, NIH, Bethesda, MD - Maryland
- TP 687 **Mass Spectrometry Based Studies on Irreversible Inhibition of Recombinant Mycobacterium Tuberculosis Hsp70 Kinase by the Marine Sponge Metabolite Ilimaquinone;** Angela Calderon¹; Johayra Simithy²; Douglas Goodwin²; Mark T Hamann³; ¹Auburn University, Auburn, AL; ²Auburn University, Auburn, Alabama; ³Medical University of South Carolina, Charleston, SC
- TP 688 **Determination of Hepatitis B Virus Infection by Means of Targeted Proteomics Strategy;** Hsing-Fen Tsai¹; He-Hsuan Hsiao¹; ¹NCHU, Department of Chemistry, Taichung, Taiwan
- TP 689 **A Key Retromer Trafficking Interactome of Toxoplasma Gondii Brought to Light by Comprehensive Proteomic Analyses;** Benoît Westermann¹; Lamba Omar Sangaré²; Agnes Hovasse¹; Tchilabalo Dilezitoko Alayi¹; Stan Tomavo²; Alain Van Dorsselaer¹; Christine Schaeffer-Reiss¹; ¹IPHC, UoS CNRS UMR 7178 Strasbourg, FRANCE; ²CNRS UMR 8204, Lille, France
- TP 690 **Proteomic Deciphering of Cystic Echinococcosis using Laser Microdissection-based Microproteomics and MALDI Imaging;** Rémi Longuespée¹; Rita Casadonte¹; Mark Kriegsmann²; Gabriel Mazzucchelli³; Edwin De Pauw⁴; Michael Becker⁵; Jörg Kriegsmann^{1,6}; ¹Proteopath GmbH, Trier, Germany; ²University of Heidelberg, Heidelberg, Germany; ³University of Liege, GIGA-Proteomics Liege, Belgium; ⁴Université de Liège, Liège, Belgium; ⁵Bruker Daltonik GmbH, Bremen, Germany; ⁶Center for Histology Cytology and Molecular Diagnostics, Trier, Germany
- TP 691 **Plasma Proteomic Changes Induced by Salmonella Typhimurium Lipopolysaccharides in an Avian Model of Inflammation ;** Balamurugan Packialakshmi¹; Rohana Liyanage¹; Jackson O Lay, Jr¹; Sarbjeet K Makkar¹; Narayan Rath²; ¹University of Arkansas, Fayetteville, AR; ²PPPSRU, USDA-ARS Fayetteville, AR
- TP 692 **Top Down Proteomic Profiling of a Hypervirulent Clinical Isolate of *Acinetobacter baumannii*;** Zack Li¹; Kelly Fulton¹; Rhonda Kuo Lee¹; Howard H Xu²; Patricia Massel¹; Susan Twine¹; Wangxue Chen¹; ¹National Research Council Canada, Ottawa, Canada; ²California State University, Los Angeles, Los Angeles, CA - California
- TP 693 **Evolutionary Dynamics of *Pseudomonas aeruginosa* Revealed by Population Proteome Analysis;** Xia Wu¹; Katherine B Hisert¹; Jayanthi Garudathri¹; Benjamin J Staudinger¹; Jimmy K Eng¹; Colin Manoil¹; Pradeep K Singh¹; James E Bruce¹; ¹University of Washington, Seattle, WA
- TP 694 **A *Plasmodium Vivax* Trophozoite-schizont Stage Transition Proteome;** D. C. Anderson¹; Stacey A. Lapp²; John Barnwell³; Mary R. Galinski⁴; ¹SRI International, Harrisonburg, VA; ²Emory Vaccine Center, Yerkes National Primate Research Center, Emory University, Atlanta, GA; ³Malaria Branch, Division of Parasitic Diseases, Centers for Disease Control and Prevention, Atlanta, GA; ⁴Emory Vaccine Center, Yerkes National Primate Research Center, Emory University; Department of Medicine, Division of Infectious Diseases, Emory University School of Medicine, Atlanta, GA

- TP 695 **Bridging Virology with Proteomics to Define Mechanisms of Cellular Immune Signaling upon Herpesvirus Infection;** Krystal K Lum¹; Benjamin A Diner¹; Joseph W Boerma¹; Ileana M. Cristea¹; ¹Princeton University, Princeton, NJ
- TP 696 **Identifying Host Factors Associated with Replicating Viral DNA;** Emigdio D Reyes^{1,2}; Katarzyna Julia Kulej^{1,2}; Daphne C Avgousti^{1,2}; Lisa Akhtar³; Daniel Bricker²; Neha Pancholi^{1,2}; Sarah A. Koniski²; Benjamin A Garcia⁴; Matthew D Weitzman^{1,2}; ¹Department of Pathology and Laboratory Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; ²Division of Cancer Pathobiology, The Children's Hospital of Philadelphia, Philadelphia, PA; ³Department of Pediatrics, Division of Infectious Diseases, The Children's Hospital of Philadelphia, Philadelphia, PA; ⁴Epigenetics program, Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA
- TP 697 **Protein-protein Interaction Network of Toll-like Receptor 4 in Macrophages with Exposure to their Agonists and External Factors;** Abu Hena M Kamal¹; Jayanta Kishor Chakrabarty¹; Saiful M Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- TP 698 **Engineering Novel Trypsin Cleavage Sites Improves Proteome Detection and PTM Recovery;** Cristal Reyna¹; Patricia A Champion²; Matthew M Champion²; ¹University of Notre Dame, South Bend, Indiana; ²University of Notre Dame, Notre Dame, Indiana
- TP 699 **Understanding Virus Mechanisms by Means of Native Mass Spectrometry;** Boris Krichel¹; Sven Falke²; Johannes Heidemann¹; Julia Lockhauserbäumer¹; Rolf Hilgenfeld³; Mathew Dunne⁴; Rob Meijers⁵; Lars Redecke³; Charlotte Utrecht^{1,6}; ¹Heinrich Pette Institute - Leibniz Institute for Experimental Virology, Hamburg, Germany; ²University of Hamburg, Hamburg, Germany; ³University of Lübeck, Lübeck, Germany; ⁴ETH Zürich, Zürich, Switzerland; ⁵EMBL Hamburg c/o DESY, Hamburg, Germany; ⁶European XFEL, Hamburg, Hamburg
- TP 700 **Cracking the Code on N-Terminal Protein Acetylation in Mycobacterium tuberculosis;** Cristal Reyna¹; Patricia Champion¹; Matthew Champion^{1,2}; ¹University of Notre Dame, Notre Dame, IN; ²The Center For Rare And Neglected Diseases, Notre Dame, IN
- TP 701 **Proteomic Analysis of the Secretome of Dengue Virus-infected Vero Cells: Characterization of the Overexpressed Viral Non-structural Protein 1 (NS1);** Chen-Ching Wu¹; Chun-Hao Huang²; Shyh- Horng Chiou²; ¹Kaohsiung Medical University, Kaohsiung City, Taiwan; ²Quantitative Proteomics Center and Graduate Institute of Medicine, Kaohsiung, TAIWAN (R.O.C.)
- TP 702 **iTRAQ Proteomic and Protein Microarray Analysis of Potential Biomarkers OipA, BabA, and SabA in Helicobacter Pylori-related Gastric Cancer;** Yu-Lin Su¹; Jyh-Chin Yang²; Lu-Ping Chow¹; ¹Institute of Biochemistry and Molecular Biology, College of Medicine, National Taiwan University, Taipei, Taiwan (R.O.C.); ²Department of Internal Medicine, Hospital and College of Medicine, National Taiwan University, Taipei, Taiwan (R.O.C.)
- PROTEOMICS: QUANTITATIVE (APPLICATION BIOLOGICAL RESEARCH)**
703 - 727
- TP 703 **Environmental Stress Induced Proteins Changes in Green Algae by Quantitative Proteomics;** Yan Gao¹; Teck Kwang Lim²; Qingsong Lin²; SAM LI¹; ¹Department of Chemistry, National University of Singapore, Singapore, Singapore; ²Department of Biological Sciences, National University of Singapore, Singapore, Singapore
- TP 704 **Proteins Associated with Olfactory Receptor Nuclear Foci;** Martin Escamilla Del Arenal¹; Fiona Clowney¹; Shujuan Tao¹; David Chen¹; Lewis M. Brown²; Stavros Lomvardas¹; ¹Columbia University, New York, NY; ²Columbia University, New York, NY
- TP 705 **Quantitative Proteomic Approach Reveals Landscape of the Regulatory Elements for Lysine 2-Hydroxyisobutyrylation Pathway;** He Huang¹; Kyle Delaney¹; Shankang Qi¹; Okwang Kwon¹; Yingming Zhao¹; ¹The University of Chicago, Chicago, IL
- TP 706 **Proteomics-based Comparison of Ionic and Nano Silver at Cytotoxic Concentrations;** Suresh Narayanasamy¹; Samantha I Wickramasekara²; Eric Sussman²; ¹U.S. Food and Drug Administration, Silver Spring, MD; ²U.S. Food and Drug Administration, Silver Spring, MD
- TP 707 **Quantitative Proteomic Analysis of PP2A-associated Proteins in BR Signaling Regulation Pathway;** Chao Liu¹; Shuo-Lei Bu²; Hao Chi¹; Zhi-Yong Wang³; Si-Min He¹; ¹ICT, CAS, Beijing, China; ²Hebei Normal University, ShiJiaZhuang, China; ³Department of Plant Biology, Carnegie Institution for Science, Stanford, USA
- TP 708 **Insights from Redox Proteomics: Focus on S-glutathionylation Stoichiometry and Redox Status of Protein Cysteines;** Jicheng Duan¹; Matthew J Gaffrey²; Hannah J. Hatchell²; Rosalie Chu²; Richard D Smith²; Brian D Thrall²; Wei-jun Qian²; ¹Pacific Northwest National Laboratory, Richland, Washington; ²Pacific Northwest National Laboratory, Richland, WA
- TP 709 **An In-depth Proteome For yeast Meiosis;** Guo Yueshuai¹; wen Fuping²; Hu Yang²; Wang Yuaning²; Wang Qian²; Yu Haiyan²; Tang Chaoming²; Sha Jiahao¹; Guo Xuejiang¹; Li Wei²; ¹Nanjing Medical University, Nanjing, China; ²Institute of Zoology, Chinese Academy of Sciences, Beijing, China
- TP 710 **Rootstock Influences Protein Profile at Different Stages of Berry Development in Grape, as Revealed by Whole Proteome Analysis using HRMS;** Smita Maske¹; Anuradha Upadhyay¹; Satisha Jogaiah¹; Akanksha Singh²; Dipankar Malakar³; Manoj Pillai³; Kaushik Banerjee¹; ¹ICAR-National Research Centre for Grapes, Pune, Maharashtra India; ²SCIEX, Gurgaon, Haryana; ³SCIEX, Gurgaon, Haryana India
- TP 711 **Proteome-wide Quantitative Profiling of Mis-Incorporation of Selenocysteine into Proteins by LC-MS Based Shotgun Proteomics;** Chunlin Hao; The Hong Kong University of Science and Technology, Hong Kong SAR, HK
- TP 712 **A Mesenchymal Stem Cells differentiation study by using SILAC and Sequence-specific DNA Affinity Purification Approaches;** Michele Puglia¹; Inigo Barrio-Hernandez¹; Blagoy Blagoev¹; ¹University of Southern Denmark, Odense, Denmark
- TP 713 **The Impact of Deyolking on Quantitative Proteomics in Zebrafish Embryos;** Fatima Rahlouni¹; Vladimir Shulaev²; Laszlo Prokai¹; ¹University of North Texas Health Science Center, Fort Worth, TX; ²University of North Texas, Denton, TX
- TP 714 **Investigation of Murine Neural Progenitor Cell to NG2 Cell Differentiation by TMT based Quantitative Proteomics;** Carmen Schoor¹; Alireza Dehghani¹; Volkmar Gieselmann¹; Dominic Winter¹; ¹University of Bonn, Bonn, Germany
- TP 715 **Proteomics- and Physiology-based Studies in Deciphering Epithelial Crosstalk Mechanism(s) Using Rhodnius prolixus as Experimental Model;** Noman Hassan¹; George Katselis²; Juan Ianowski²; ¹University of Saskatchewan, Saskatoon, SK; ²University of Saskatchewan, Saskatoon, Canada



- TP 716 **Age Dependent Protein Expression in Drosophila Models of Neurodegeneration;** Chris Brown¹; Jonathan C Trinidad¹; David E Clemmer¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- TP 717 **Quantitative Proteome Profiling of Marinobacter sp. CP1 enriched from Microbial Fuel Cell Biocathode MCL;** W. Judson Hervey, IV¹; Zheng Wang¹; Brian J. Eddie¹; Anthony P. Malanoski¹; Baochuan Lin¹; Sarah M. Strycharz-Glaven¹; ¹Naval Research Laboratory, Center for Bio/Molecular Science & Engineering, Washington, DC
- TP 718 **Novel Top-down Quantitative LC/MS Strategy Reveals New Insights into Molecular Heterogeneity In Skeletal Muscle;** Ziqing Lin¹; Liming Wei^{1,2}; Yutong Jin¹; Wenxuan Cai¹; Zachery Gregorich¹; Gary M Diffe¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²Fudan University, Shanghai, China
- TP 719 **Combined Discovery- and Targeted-based Proteomic Analysis of Tumor-Associated Antigen Peptides Derived from MAGE Proteins;** Darshit Shah¹; Xunbao Duan²; MacDonald Douglas²; Robert Salzler²; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY; ²Regeneron Pharmaceuticals, Tarrytown, NY
- TP 720 **Fast MS/MS Data Acquisition without Dynamic Exclusion Enables Precise and Accurate Quantification of Proteome;** Yichu Shan; , dalian, liaoning
- TP 721 **A Comparison of Isobaric Labeling with MS1-XIC Quantitation using a Two-Proteome Model;** David Mccaskill¹; Trent Oman¹; Tao Xu¹; Jeffrey R Gilbert¹; ¹Dow AgroSciences, Indianapolis, IN
- TP 722 **Application of Mass Spectrometry Profiling to Establish Brusatol as an Inhibitor of Global Protein Synthesis;** Taylor Ma¹; Steffan Vartanian²; James Lee²; Peter M Haverty²; Donald S Kirkpatrick²; Kebin Yu²; David Stokoe²; ¹Genentech, Inc., South San Francisco, CA; ²Genentech Inc, South San Francisco, CA
- TP 723 **Proteomics Profiling of Parental and mAb-producing CHO-derived Cell Lines to Facilitate Optimization of mAb Production;** Yee Jiun Kok¹; Ally Lau¹; Daniel Ng¹; Lu Zheng¹; Yuansheng Yang¹; Xuezhi Bi¹; ¹Bioprocessing Technology Institute, Singapore
- TP 724 **Quantitative Analysis of Chromatin Proteome Remodeling Mediated by SWI/SNF Complexes;** Zhiping Wu¹; Eun-Ah Cho²; Haiyan Tan³; Haifeng Yang²; Junmin Peng³; ¹ST. Jude, Memphis, TN; ²Thomas Jefferson University, Philadelphia, PA; ³St. Jude Children's Research Hospital, Memphis, TN
- TP 725 **Use of Variant Proteomics to Inform Genomic Searches for Novel Targets in Glioma;** Ekaterina Mostovenko¹; Melinda Rezeli²; Akos Vegvari¹; Gyorgy Marko-Varga²; Yanhong Liu³; E. Susan Amirian³; Melissa L Bondy³; Carol L Nilsson¹; ¹UTMB Galveston, Galveston, TX; ²Lund University, Lund, Sweden; ³Dan L. Duncan Cancer Center, Houston, TX
- TP 726 **Determining Isotope Enrichment in Heavy Water Labeling;** Jayant Avva¹; Kwangwon Lee²; Takhar Kasumov³; Rovshan Sadygov¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX; ²Northeast Ohio Medical University, Rootstown, OH; ³Northeast Ohio Medical University, Rootstown, OH
- TP 727 **Quantitative MS Investigation of the Effect of Amyloid-Beta on the Proteome Of Neuronal Cells;** Maria L Indeykina^{1,2,3}; Evgeny P Barykin⁴; Alexey S Kononikhin^{2,3,5}; Vladimir Mitkevich⁴; Igor A Popov^{2,3}; Sergey Kozin⁴; Alexander A Makarov⁴; Eugene Nikolaev²; ¹Emanuel Institute of Biochemical Physics, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; ⁴Engelhardt Institute of Molecular Biology, Moscow, Russia; ⁵Research Center for Obstetrics and Gynecology, Moscow, Russia
- SMALL MOLECULES: QUANTITATIVE ANALYSIS (ANIMAL, PLANT/INSECT, AND METHODOLOGY)**
728 - 762
- TP 728 **Quantitative Measurement of Carbidopa and Levodopa in Rat Plasma via HPLC with Tandem Mass Spectrometry;** Jingduan Chi¹; Yonghua Ling¹; Mofikoya Melissa¹; Fumin Li¹; ¹PPD, Middleton, WI
- TP 729 **A Sensitive LC-MS-MS Method for Quantitation of Buprenorphine in Rat Brain Cerebrospinal Fluid;** Fengying Zhu¹; Perry (Peixin) Cao¹; Ryan Turncliff¹; ¹Alkermes, Inc, Waltham, MA
- TP 730 **Challenges and Solutions in the Bioanalysis of Sulprostone, a Prostaglandin E2 Analogue, in Rat and Monkey Plasma using LC-MS/MS;** Yifan Shi¹; Shefali Patel¹; Naidong Weng¹; ¹Janssen Research and Development, Spring House, PA
- TP 731 **A Novel Determination for Menthol in Rat Plasma using Salting-Out LLE and Derivatization Coupled with LC-MS/MS Detection;** Mingluan Chen¹; Milton Furtado¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- TP 732 **Ultra Sensitive Method for Pre-clinical Quantification of Methacholine in Biological Matrices using SPE-HILIC Tandem Mass Spectrometry;** Anders Lundqvist; AstraZeneca Gothenburg, Gothenburg, Sweden
- TP 733 **Development and Validation of a Method to Quantitate Bisphenol AF in Rodent Plasma and Amniotic Fluid by LC/MS/MS;** Bradley Collins¹; Felicia Hubbard²; Kristin L. Aillon²; Joseph W. Algaier²; Suramya Waidyanatha¹; ¹National Institute of Environmental Health Sciences, Research Triangle Park, NC; ²MRIGlobal, Kansas City, MO
- TP 734 **Simultaneous Determination of Benzocaine, N-acetyl Benzocaine, and Tetracaine in Rabbit Plasma using High Performance Liquid Chromatography-Mass Spectrometry;** Wuyi (Charlie) Zha¹; Runlan Huo¹; Mohamed Osman¹; Xinping Fang²; Xin Zhang²; ¹XenoBiotic Laboratories, Inc. WuXi AppTec Inc Plainsboro, NJ; ²WuXi AppTec Co., Shanghai, China
- TP 735 **Validation of a Method for Quantification of DMSO in Equine Urine using Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry;** Matilda Salomonsson^{1,2}; Lena Ekman³; Mikael Hedeland³; Ulf Bondesson^{2,3}; ¹The National Veterinary Institute (SVA), Uppsala, -; ²Uppsala University, Uppsala, Sweden; ³The National Veterinary Institute (SVA), Uppsala, Sweden
- TP 736 **A Robust LC/MS/MS Method for Quantitation of 2-morpholinoethanesulfonic acid (MES) in Dog and Rabbit Plasma;** Todd Baughman; Covance, Durham, NC
- TP 737 **Analysis of Mycotoxins in Coix Seed using a Prototype Tandem Quadrupole Mass Spectrometer;** Kerri Smith¹; Kelly B Doering¹; Mark Wrona¹; Giorgis Isaac¹; Jimmy Yuk¹; Sukhdev Bangar²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA
- TP 738 **Quantification of Biogenic Amines from Single Drosophila Cells by Direct MALDI-TOF MS;** Max Diesner¹; Susanne Neupert¹; ¹Biocenter Cologne, University of Cologne 50674 Cologne, Germany
- TP 739 **CBD/THC Quantitative Analysis with Direct Analysis in Real Time-Mass Spectrometry (DART-MS);** Bohui Lv¹; William Hoffmann²; Glen P Jackson¹; ¹West Virginia University, Morgantown, WV; ²Oak Ridge National Laboratory, CNMS Oak Ridge, TN
- TP 740 **A Combined MRM and SIM Method for Direct Quantitative Determination of Amino Acids in Various Samples on LC/MS/MS;** Zhe Sun¹; Jie Xing¹; Pei Yee Khoo²; Zhaoqi Zhan¹; ¹Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; ²School of Physical & Mathematical Sciences, Nanyang Technological University Singapore, *Intern student
- TP 741 **Mass Spectrometry-Guided Refinement of Chemical Energy Buffers;** Ting-Ru Chen¹; Pawel Lukasz Urban²;

- ¹National Chiao Tung University, Hsinchu, Taiwan;
²Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.)
- TP 742 **Obtain sub-ng/mL Levels for Steroids using a Simple, One-step Derivatization and a Novel, High Efficiency EI Source;** Tim Conjelko¹; Stephan Baumann¹; Matthew Curtis¹; ¹Agilent Technologies, Santa Clara, CA
- TP 743 **Novel SPE Extraction Method for Sensitive and High Throughput Quantitative Analysis of Phosphorothioate Oligonucleotides in Human Plasma Using LC-MS/MS;** Yuhuan Ji¹; Qian Liu¹; Qian Li¹; Ji Chengjie¹; Laixin Wang²; ¹NovaBioAssays, LLC, Woburn, MA; ²NovaBioAssays, LLC, Woburn, MA
- TP 744 **Quantitation of Four Chiral Drug Compounds Simultaneously Using Normal Phase LC-MS/MS Equipped With an APPI Ion Source;** Min Huang¹; Zhongping (John) Lin¹; ¹Frontage Laboratories, Exton, PA
- TP 745 **The Use of Perchloric Acid as a Problem Solving Precipitating Agent to Overcome Method Development Issues;** Pierre-Yves Caron¹; Nicolas Jean¹; Nadine Lafontaine¹; Louis-Charles Boisvert¹; Sylvain Lachance¹; Nadine Boudreau¹; Clark Williard¹; ¹inVentiv Health, Québec, Canada
- TP 746 **A Novel Approach for Reducing the Isotopic Distribution Impact during Quantitation of Analyte by LCMSMS using Quadratic Regression Fit;** Nathalie Pelletier¹; Genevieve Emond¹; Sylvain Lachance¹; Nadine Boudreau¹; Clark Williard¹; ¹inVentiv Health, Québec, Canada
- TP 747 **Monitoring and Quantitating Genotoxic Impurities using Mass Detection and UV – Sensitive Analysis Aryl Sulfonic Acid Esters;** Mark Wrona¹; Janet Hammond²; Jayne Kirk²; Sean McCarthy¹; Hillary Hewittson¹; Margaret Maziarz¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, UK
- TP 748 **Development of a Low Volume Quantitative Plasma Analysis Method Using a Flexible Capillary Microsampling Technique;** Larry Mallis¹; Wei Zhang¹; Li Yuan¹; Zhongping (John) Lin¹; ¹Frontage Laboratories, Exton, PA
- TP 749 **An Investigation on the Impact on Drug Stability in Biological Matrix when Stored in Multiple Tubes;** Nader Youssef¹; John Chapdelaine¹; Weixing Sun¹; Asvinkumar Patel¹; Zhao Heng Ge¹; Adrien Musuku¹; ¹Pharmascience, Montreal, Canada
- TP 750 **Simultaneously Determination of the Enantiomers of Ketorolac in Human Plasma by Atmospheric Pressure Chemical Ionization LC/MS/MS;** Vince Windisch¹; Feng Liang¹; Allan Xu¹; ¹Keystone Bioanalytical Inc, North Wales, PA
- TP 751 **Trace Analysis of Potentially Mutagenic Impurities in Pharmaceutical Substances by Electron Ionization LC/MS (EI-LC/MS) with Supersonic Molecular Beams;** Christine Fisher¹; Ryan Cohen¹; Renee Dermenjian¹; ¹Merck & Co., Rahway, NJ
- TP 752 **Expanding Horizons in Real Time Analysis: Dual Polarity SIFT-MS;** Murray J McEwan^{1,2}; David Hera²; Harry Gower²; Vaughan S Langford²; Thomas I McKellar²; Daniel B Milligan²; ¹University of Canterbury, Christchurch, Canterbury; ²Syft Technologies Ltd, Christchurch, New Zealand
- TP 753 **Development of LC/MS/MS Method for Screening and Quantitation of 49 Synthetic Dyes in Textiles under Restricted Substance List (RSL);** Yin Ling Chew¹; Jie Xing¹; Guan Seng, Leonard Lim²; Zhaoqi Zhan¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore; ²School of Physical & Mathematical Science, Nanyang Technological University, Singapore
- TP 754 **Isolation, Characterization and Color Stability of natural blue pigments;** Andrew G Newsome¹; Luying Chen¹; Cathy A Culver²; Richard B van Breemen¹; ¹University of Illinois at Chicago, Chicago, IL; ²Pepsi-Cola Company, Hawthorne, NY
- TP 755 **Selective Enrichment of Flavonoids Using Pegylated Graphene Oxide and MALDI-TOF MS;** Jaesung Lee; Konkuk University, Seoul, South Korea
- TP 756 **Development of a Sensitive Supercritical Fluid Chromatography (SFC)-MS/MS Method for the Analysis of Potential Genotoxic Impurities of Ondansetron;** Jennifer Simeone¹; Paula Hong¹; ¹Waters Corporation, Milford, MA
- TP 757 **Development and Testing of a Gas Generator for Odour Transmission over Data Networks;** Stamatis Giannoukos¹; Jeremy Smith²; Alan Marshall²; Stephen Taylor²; ¹University of Liverpool, Liverpool, Please Select; ²University of Liverpool, Liverpool, United Kingdom
- TP 758 **Novel Applications of Paired Ion Electrospray Ionization Mass Spectrometry (PIESI-MS) for Sensitive Analysis of Anionic Compounds;** Hongyue Guo¹; Daniel W Armstrong¹; ¹University of Texas at Arlington, Arlington, TX
- TP 759 **Parallel Reaction Monitoring and Selected Reaction Monitoring Exhibit Comparable Analytical Performance in Quantitative Analysis of Cannabinoid;** Xiaolei Xie¹; Thomas Carrell¹; Marta Kozak¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 760 **A Simple Systematic Strategy for Rapid Development of High-throughput and Reliable LC-MS/MS Assays for Regulated Bioanalysis;** Long Yuan; Bristol-Myers Squibb, Princeton, NJ
- TP 761 **Commutability of LCMSMS Assays: Calibration by Internal or External Standardization?** R. Brent Dixon; Physician's Choice Laboratory Services, Rock Hill, SC
- TP 762 **Evaluation of an Innovative High-Throughput Online Solid Phase Extraction Tandem Mass Spectrometry System for Bioequivalence Studies;** Jinhui Zhang¹; Patrick J. Faustino¹; ¹FDA, Silver Spring, MD
- TOP DOWN PROTEIN ANALYSIS (METHODOLOGY)**
763 - 775
- TP 763 **The National Resource for Translational and Developmental Proteomics offers novel opportunities for training and accelerated research in top-down proteomics;** Neil L Kelleher¹; Caroline J DeHart¹; Ryan T Fellers¹; Richard D LeDuc¹; Paul M Thomas¹; ¹Northwestern University, Evanston, IL
- TP 764 **Application of Spectral Counting for Top-down Proteomics Comparisons;** Lucia Geis-Asteggian¹; Nathan Edwards²; Suzanne Ostrand-Rosenberg³; Catherine Fenselau¹; ¹University of Maryland, College Park, MD; ²Georgetown University Medical Center, Washington, DC; ³University of Maryland, Baltimore County Baltimore, MD
- TP 765 **Increased Fragmentation Efficiency in Middle-down Protein Analysis using Different Collision Gases in a Modified Q-TOF Mass Spectrometer;** Christian Klein¹; Alex Mordehai¹; Mark Werlich¹; William E Barry¹; ¹Agilent Technologies, Santa Clara, CA
- TP 766 **Protein Supercharging for Enhanced Top-Down Analysis with HCD MS/MS;** Natalia Gasilova¹; Kristina Srzentic²; Yuri Tsybin³; Hubert H Girault⁴; ¹EPFL, Sion, Switzerland; ²EPFL, Lausanne, Switzerland; ³Spectroswiss Sàrl, Lausanne, Switzerland; ⁴EPFL, Sion, Switzerland
- TP 767 **Difference Mass Spectra for De novo Identification of N- and C-terminal Sequences of Intact Proteins;** Harsha Gunawardena¹; Dhanshi Bagal¹; Daryl Bulloch¹; Ping Cao¹; David Chow¹; Eddie Kast¹; Matthew Rardin¹; Nik Sharkov¹; Peter Grandsard²; ¹Amgen, Inc. South San Francisco, CA; ²Amgen, Thousand Oaks, CA
- TP 768 **Top-down Targeted Proteomics Reveals Novel Molecular Mechanism in Sarcopenia;** Zachery Gregorich¹; Ying Peng²; Wenxuan Cai²; Yutong Jin²; Liming Wei³; Albert Chen²; Susan McKiernan²; Judd Aiken⁴; Richard Moss²; Gary Diffe²; Ying Ge²; ¹UW Madison, Madison,



- WI; ²University of Wisconsin Madison, Madison, WI; ³Fudan university, shanghai, China; ⁴University of Alberta, Edmonton, Canada
- TP 769 **Optimisation of intact Protein Sequencing through Testing Thousands of EThCD/ETciD MS/MS Fragmentation Conditions;** Pavel Shliha¹; Derek Bailey²; Vladimir Gorshkov¹; Ole N. Jensen¹; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; ²Thermo Fisher Scientific, San Jose, CA
- TP 770 **Development of Mass Spectrometry-based Methods for Quality Assessment of Recombinant Proteins;** Rosa I Viner¹; Nan Liu²; Seema Sharma¹; Sergei I Snovida³; Krishna Vatter³; David M Horn¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Life Technology, South San Francisco, CA; ³Thermo Fisher Scientific, Rockford, IL
- TP 771 **Higher-order Structure Determines the Native ETD Fragmentation Behavior of Proteins and Complexes;** Frederik Lermite¹; Mateusz Krzysztof Łacki²; Albert Konijnenberg¹; Dirk Valkenburg³; Anna Gambin²; Frank Sobott¹; ¹University of Antwerp, Antwerpen, Belgium; ²University of Warsaw, Warsaw, Poland; ³VITO, Mol, Belgium
- TP 772 **Native Top-down Mass Spectrometry of Tau Proteins;** Piriya Wongkongkathep¹; Michael Nshanian¹; Michael Ehrmann²; Gal Bitan¹; Joseph A Loo¹; ¹UCLA, Los Angeles, CA; ²University of Duisburg-Essen, Essen, Germany
- TP 773 **Mapping p53 Proteoforms by Native and Denaturing Top-down Mass Spectrometry;** Caroline J DeHart¹; Luca Fornelli¹; Owen Skinner¹; Philip D Compton¹; Paul M Thomas¹; Galit Lahav²; Jeremy Gunawardena²; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL; ²Harvard Medical School, Boston, MA
- TP 774 **High-throughput Top Down Proteomics of HeLa cell lysates using UVPD;** Timothy Cleland¹; Ryan Parker²; Jennifer S Brodbelt¹; ¹University of Texas Austin, Pflugerville, TX; ²University of Texas at Austin, Austin, TX
- TP 775 **Quantitative Top Down Proteomics in Translational Research: Markers for Rejection in Peripheral Blood Following Kidney Transplantation;** Timothy Toby¹; John Savaryn¹; Bryan P Early¹; Paul M Thomas¹; Ryan T Fellers¹; Luca Fornelli¹; Joseph B Greer¹; Richard D Leduc¹; Ioanna Ntai¹; Zheng J Zhang²; John Friedewald²; Daniel Salomon³; Michael M Abecassis²; Neil L Kelleher¹; Philip D Compton¹; ¹Northwestern University, Evanston, IL; ²Northwestern Feinberg School of Medicine, Chicago, IL; ³Scripps Center for Organ and Cell Transplantation, La Jolla, CA

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

Ambient Ionization: Fundamentals and Instrumentation (Probes, Paper Spray, DESI/ESI, Tissue/Tools).....	001 - 029
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Biomarkers: Discovery (Part 1).....	062 - 088
Biomarkers: Quantitative Analysis (Part 2).....	089 - 116
Carbohydrates (Glycans).....	117 - 138
Disease Biomarkers.....	139 - 153
Drug Discovery/DMPK/ADME (General).....	154 - 177
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Environmental Analysis: Water Quality.....	190 - 206
Food Safety: Other Contaminants (Part 1).....	207 - 235
Food"omics" MS Characterization of Food and Nutritional Supplements (Part 2).....	236 - 252
Forensics (Part 2).....	253 - 278
GCMS: Instrumentation and Applications (Instrumentation-New Developments).....	279 - 293
Glycoproteins (Tandem MS, Separations, and Automation/Software).....	294 - 313
H/D Exchange: Hardware, Software and Methodology.....	314 - 327
H/D Exchange: Protein Structure/Function (Part 1).....	328 - 336
ICP and Isotope Ratio MS: Elemental.....	337 - 341
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Informatics: Algorithms and Statistical Advances.....	365 - 389
Informatics: Workflow and Data Management.....	390 - 405
Instrumentation: Mini/Portable/Fieldable MS.....	406 - 425
Instrumentation: New Developments in Ionization and Sampling (Sampling).....	426 - 438
Ion Mobility: Fundamentals.....	439 - 463
Ion Structure/Energetics.....	464 - 482
LC-MS: Sample Preparation (Part 1).....	483 - 504
Lipids: Profile Analysis.....	505 - 536
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Metabolomics: Untargeted Metabolite Profiling (Animal/Human/Other).....	550 - 574
Nanoscale and Microfluidic Separations and MS.....	575 - 586
Plant 'omics'.....	587 - 613
Protein Therapeutics: Quantitative Analysis.....	614 - 650
Proteomics: New Approaches (Global).....	651 - 674
Proteomics: Quantitative (Labeling/Tagging/MS/ Quantitation).....	675 - 704
Small Molecules: Quantitative Analysis (Part 1).....	705 - 728

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION (PROBES, PAPER SPRAY, DESI/ESI, TISSUE/TOOLS)

001 - 029

- WP 001 **Development of a DIP-APPI-IM-qTOF-MS;** Simeon Horst¹; Oliver Schmitz¹; ¹Universität Duisburg Essen, Essen, Germany
- WP 002 **Development of a DIP-ESI-MS for Drug Analysis;** Claudia Lenzen¹; Oliver Schmitz¹; ¹Universität Duisburg Essen, Essen, Germany
- WP 003 **Monolith Dip-It: A Bifunctional Device for Increasing the Sensitivity of Direct Analysis in Real Time;** Li Xianjiang¹; Yu Bai¹; Liu Huwei¹; ¹Peking University, Beijing, China
- WP 004 **Inert - Atmospheric Solid Analysis Probe: A New Fast and Easy Way to Characterize Air Sensitive Compounds by Mass Spectrometry;** Mathilde Farenc^{1,2,3}; Carlos Afonso^{2,3}; Pierre Giusti^{1,3}; ¹TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; ²Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; ³TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, France,

- WP 005 **Applications and Fundamentals of Swab Touch Spray – Mass Spectrometry;** Alan K. Jarmusch^{1,2}; Valentina Pirro^{1,2}; R. Graham Cooks^{1,2}; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Center for Analytical Instrumentation Development, West Lafayette, IN
- WP 006 **Coupling Paper Microfluidics with Paper Spray Mass Spectrometry for Improved Versatility and Analytical Performance;** Ian Murray¹; Glenn Walker¹; Michael Bereman¹; ¹North Carolina State University, Raleigh, NC
- WP 007 **In situ Separation and Analysis of Lipids by Paper Spray Ionization Mass Spectrometry;** Sangwon Cha¹; Purum Kim¹; ¹Hankuk Univ. Foreign Studies, Yongin, South Korea
- WP 008 **High-Throughput Copper-Catalysts Screening and Their Catalytic Activity Studies Using Paper Spray Mass Spectrometry;** Yajun Zheng¹; Xuan Wang¹; Teng Wang¹; Yang Haijun²; Zhiping Zhang¹; ¹Xi'an Shiyu University, Xi'an, China; ²Tsinghua University, Beijing, China
- WP 009 **Molecular Ionization at Low Voltage from One-Dimensional Nanostructures;** Rahul Narayanan; Indian Institute of Technology, Chennai, Tamilnadu, India, Chennai, Tamilnadu
- WP 010 **Dehydrogenation of Tetrahydroquinolines in Corona Discharge Plasma under Ambient Conditions using Graphite-Coated Hydrophobic Paper Surface;** Kathryn Davis¹; Abraham Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 011 **Mass Spectrum Real-Time Online Optimizing Paal-Knorr Spary Reaction Temperature;** XingPing Zeng¹; Peng Zhou¹; Huanwen Chen²; ¹East China Institute of Technology, Nanchang, China; ²East China University of Technology, Nanchang, Mainland
- WP 012 **Direct and Rapid Detection of Drugs in Urine by Extractive Electrospray Ionization Mass Spectrometry;** Peng Zhou¹; Tenggao Zhu¹; Yongzi Liu²; Huian Zhao²; Huanwen Chen³; ¹East China Institute of Technology, Nanchang, China; ²Jiangxi of Forensic Science Institute, Nanchang, China; ³East China University of Technology, Nanchang, Mainland
- WP 013 **Coaxial Extractive Electrospray Ionization Mass Spectrometry;** Kenneth D Swanson¹; Steven L Reeber¹; Gary L Glish¹; ¹University of North Carolina, Chapel Hill, NC
- WP 014 **Generating Radical Cations of Aromatic Hydrocarbons through Reactive ESI Using the Single-Probe;** Rachel Vowcicefski¹; Ning Pan²; Zhibo Yang²; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Dept. of Chem & Biochem Norman, OK
- WP 015 **Pinpointing the Source of Droplet Reactivity in Contained-electrospray Ionization;** Dmytro Kulyk¹; Abraham Badu-Tawiah¹; ¹Ohio State University, Columbus, OH
- WP 016 **Solvent Assisted Inlet Ionization of Airborne Nanoparticles;** Andy Horan¹; Murray V Johnston¹; ¹University of Delaware, Newark, Delaware
- WP 017 **Ionization Efficiency Comparison of ESI, SAI, and vSAI Using Compounds with Different Surface Activities;** Madeline Fenner¹; Charles N McEwen²; ¹University of the Sciences, Philadelphia, PA; ²University of the Sciences in Philadelphia, Philadelphia, PA
- WP 018 **Effects of Volatile Anions and Cations as Spray Solvent Additives on the DESI-MS Analysis of Proteins;** Andre Venter¹; Elahe Honarvar¹; Wisam Alisawi¹; ¹Western Michigan University, Kalamazoo, MI
- WP 019 **Top-down DESI-UVPD of Proteins and Lipopolysaccharides on Polyvinylidene Difluoride Membranes;** Dustin Klein¹; Clara Feider¹; Livia S Eberlin¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX

- WP 020 **DART Mass Spectrometry and Emission Spectra of Various DART Gas Sources;** William A. Harris¹; Johnny K Ho¹; Douglas B Henderson¹; ¹Northrop Grumman, Linthicum Heights, MD
- WP 021 **Ambient MS Based Analytical Platform for Rapid Identification of Brain Cancer Tumor Tissues;** Igor A Popov^{1,2}; Evgeny Zhvansky^{1,2}; Nikita Levin¹; Vsevolod Shurkhay³; Denis Bormotov¹; Maria Indeykina^{2,4}; Alexey S Kononikhin^{2,4}; Yuri Kostyukovich^{2,4}; Evgeny Kukaev^{1,2}; Alexander Potapov³; Eugene Nikolaev²; ¹Moscow Institute of Physics and Technology, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Burdenko Neurosurgical Institute, Moscow, Russian Federation; ⁴Emanuel Institute of Biochemical Physics, Moscow, Russia
- WP 022 **Assessment of Atmospheric Pressure Surface Mass Spectrometries for Improved Characterization and Imaging of Medical Devices;** Felicia M Green¹; Adam Taylor²; Rory Steven²; Elzbieta Gurdak²; Josephine Bunch²; ¹National Physical Laboratory, Teddington, Middlesex; ²National Physical Laboratory, Teddington, UK
- WP 023 **Liquid Microjunction Sampling for the Analysis of Proteins from Thin Tissue Sections;** Rian Griffiths¹; Elizabeth C Randall¹; Helen J Cooper¹; ¹The University of Birmingham, Birmingham, UK
- WP 024 **Ambient Bio-Molecular Mass Spectrometric Imaging with Subcellular Spatial Resolution;** Jae Young Kim¹; Eunsoek Seo¹; Hyunmin Kim²; Dong-Kwon Lim³; Dae Won Moon¹; ¹Department of New Biology, DGIST, Daegu, South Korea; ²Nano and Energy Research Division, DGIST, Daegu, South Korea; ³KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea
- WP 025 **Spot Size, Sensitivity, and Fit for Purpose: Comparative Analysis of Extractive Analysis Techniques;** Mariam S Elnaggar; *Prosolia, Inc., Indianapolis, IN*
- WP 026 **Point-of-Care Tissue Analysis with Specificity for C=C Bond Lipid Isomers;** Ran Zou^{1,2}; Xiao Wang^{1,2}; Leelyn Chong^{1,2}; Yuan Su^{1,2}; Xiaoxiao Ma^{1,2}; Jessica Page^{1,3}; Riya Shi^{1,3}; Yu Xia^{1,4}; Zheng Ouyang^{1,2}; ¹Purdue University, West Lafayette, IN; ²Biomedical Engineering, Purdue University West Lafayette, IN; ³School of Veterinary Medicine, Purdue University, West Lafayette, IN; ⁴Chemistry Department, Purdue University West Lafayette, IN
- WP 027 **Robotic Surface Analysis Mass Spectrometry (RoSA-MS) for Automated Ambient Sampling of Highly-Curved Three-Dimensional Surfaces;** Martin R L Paine¹; Rachel V Stryfller²; Anyin Li¹; Jake Huckaby³; Alexander S Lambert¹; Ruffin J White¹; Henrik I Christensen¹; Facundo M Fernández¹; ¹Georgia Institute of Technology, Atlanta, GA; ²The Coca Cola Company, Atlanta, GA; ³Energid, Boston, MA
- WP 028 **Ambient Robotic Mass Spectrometry via Cross Platform Synchronization;** Jason Wu; *Georgia Tech, Atlanta, Georgia*
- WP 029 **Development of a Field-Free Ambient Pressure Desorption Thermal Ionization Probe;** Josh Swider¹; Dale Chatfield¹; ¹San Diego State University, San Diego, CA
- WP 030 **Protease-Containing Membranes For Controlled Digestion of Antibody Cocktails and Enhancement of Monoclonal Antibody Sequencing;** Yongle Pang¹; Merlin Bruening¹; ¹Department of Chemistry, Michigan State University, East Lansing, MI
- WP 031 **Validation of Originator Sequences by Antibody Domain Mass Determination and Top-Down Sequencing;** Anja Resemann¹; Wolfgang Jabs¹; Anja Wiechmann¹; Elsa Wagner²; Colas Olivier²; Waltraud Evers¹; Eckhard Belau¹; Lars Vorwerg¹; Catherine Evans¹; Alain Beck²; Detlev Suckau¹; ¹Bruker Daltonic GmbH, Bremen, Germany; ²Centre d'Immunologie Pierre-Fabre, St. Julien-en-Genevois, France
- WP 032 **Distinguishing Leucine and Isoleucine Residues in de novo Sequencing of mAbs using Nano LC-MSn: A Potential to Replace Edman Degradation;** Dhanashri Bagal¹; Ping Cao²; Eddie Kast²; ¹Amgen, South San Francisco, CA; ²Amgen, Inc. South San Francisco, CA
- WP 033 **High Throughput Antibody de novo Sequencing and Its Utility in Biopharmaceutical Discovery;** Kadir Ilker Sen¹; Darryl Davis¹; Wilfred Tang²; Marshall Bern²; Chris Becker²; ¹Janssen Research and Development, Spring House, PA; ²Protein Metrics Inc., San Carlos, CA
- WP 034 **Automated Antibody Sequencing Software;** Wilfred Tang¹; Marshall Bern¹; Chris Becker¹; Kadir Ilker Sen²; ¹Protein Metrics Inc., San Carlos, CA; ²Janssen Research and Development, Spring House, PA
- WP 035 **Rapid Quantitation of IgG after Digestion at Elevated Temperature with a Novel Trypsin Reagent;** Michael Rosenblatt¹; Daniel S Spellman²; Sergei Saveliev¹; Kevin P Bateman²; Marjeta Urh¹; ¹Promega Corp, Madison, WI; ²Merck & Co., Inc., West Point, PA
- WP 036 **Comparison of Various LC/MS Methods for Label-free Relative Quantitation of Site-specific Glycosylation of a Monoclonal Antibody;** Pilsoo Kang¹; Jianmei Kochling¹; ¹Sanofi Genzyme, Framingham, MA
- WP 037 **Minimizing Method-induced Modifications in the Complementarity Determining Regions (CDRs) of Antibodies to Ensure Optimal Understanding of Product Quality Attributes;** Jennifer Ide¹; Elaine Stephens²; Michelle A English²; Jason C Rouse²; Lisa A Marzilli²; ¹Pfizer, Andover, MA; ²Pfizer, Inc. Andover, MA
- WP 038 **A Method Comparison for Quantifying Trisulfides in Monoclonal Antibodies: Non-Reduced Peptide Mapping LC-MS vs. Hydrophilic Interaction Chromatography-Charged Aerosol Detection;** Christopher Cornell; *Genentech, South San Francisco, CA*
- WP 039 **Impact of Fc N-Glycan Sialylation on IgG Structure;** Zhongqi Zhang^{1,1}; Bhavana Shah¹; Jason Richardson¹; ¹Amgen, Inc., Thousand Oaks, CA
- WP 040 **Evaluation of a Rapid Method for Deamidation Profiling of Monoclonal Antibodies Suitable for Early Molecular Selection in Drug Discovery;** Heather DeGruttola¹; Elaine Stephens¹; Michelle English¹; Keith A Johnson¹; Anja Wiechmann²; Guillaume Tremintin³; Jason Wood⁴; Wolfgang Jabs²; Lisa A Marzilli¹; Jason Rouse¹; ¹Pfizer, Inc. Andover, MA; ²Bruker Daltonic GmbH, Bremen, Germany; ³Bruker Daltonics, Fremont, CA; ⁴Bruker Daltonics, Inc., Billerica, MA
- WP 041 **The Effect of Sialylation of IgG's N-Glycans on FcRn Binding;** Jake Pawlowski¹; Adriana Bajardi-Taccioli²; Damian Houde²; Marina Feschenko²; Igor A Kaltashov³; Tyler Carlage²; ¹UMASS Amherst, Amherst, Massachusetts; ²Biogen Inc., Cambridge, MA; ³University of Massachusetts, Amherst, MA
- WP 042 **Characterization of Relative N-Glycan Occupancy in Antibodies using Mass Spectrometry;** Ekaterina G. Deyanova¹; Yun Wang¹; Richard Huang¹; Guodong Chen¹; ¹Bristol-Myers Squibb, Princeton, NJ
- WP 043 **Analysis of O-linked Glycan Released from Biopharmaceuticals by using a Chemical Reaction and ASDP-incorporated Curved Field Reflectron;** Shuuichi Nakaya¹; Yuzo Yamazaki¹; ¹Shimadzu Corporation, Kyoto, Japan
- WP 044 **Building a High Confidence, Quantitative O-glycopeptide Profile for IgA;** Amol Prakash¹; Shadab Ahmad¹; Scott M Peterman²; Julian A Saba³; Chu-Wei Kuo⁴; Kay-Hooi Khoo⁴; Rosa I Viner³; ¹Optys Tech Corporation,

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- Brighton, MA; ²Thermo Scientific BRIMS, Cambridge, MA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Academia Sinica, Taipei, Taiwan
- WP 045 **A Novel Approach to Disulfide Bond Reduction in Antibodies using Electrochemistry with Online Mass Spectrometry;** Arielle Verdi¹; Laurent Rieux²; Martin Eysburg²; Andrew Milinichik¹; Xin Cheng¹; Earl Albone¹; ¹Morphotek Inc., Exton, PA; ²Antec LLC, Boston, MA
- WP 046 **A Novel Method for Rapid Quantitative Determination of Total Free Sulfhydryls of an Antibody Fragment;** Weitao Jia¹; Qian Cai¹; Jennifer Zhang¹; ¹Genentech Inc, South San Francisco, CA
- WP 047 **Middle-down Approach for Monitoring Monoclonal Antibody Variants and Deglycosylation;** Shanhua Lin¹; Zoltan Szabo¹; Yury Agroskin¹; Terry Zhang²; Jonathan L Josephs²; Xiaodong Liu¹; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, San Jose, CA
- WP 048 **Synthesis of Glycopeptides to be Used as Internal Standards for MALDI-MS Analysis of Tryptic Digestion Products from Antibodies;** Rini Roy¹; Ronald Domalaon¹; Frank Schweizer¹; Helene Perreault²; ¹University of Manitoba, Winnipeg, Canada; ²University of Manitoba, Winnipeg, MB
- WP 049 **Detection and Characterization of Stress-induced Oxidation and Deamidation on Vulnerable Sites of Etanercept Products;** Li-Juan Huang¹; Shu-Hui Chen¹; ¹Chemistry Dept. NCKU, Tainan, Taiwan (R.O.C.)
- WP 050 **Rapid Evaluation of Domain-specific PTMs in mAbs and Drug Conjugations in ADCs via a New Middle-down Proteomics Tool;** Charles Nwosu¹; Bisola Asaolu²; John Piscitelli²; May Zhu²; ¹Takeda Pharmaceuticals International Inc., Cambridge, MA; ²Takeda Pharmaceutical International Inc., Cambridge, MA
- WP 051 **Antibody Characterization Enabled by Automated Affinity Purification, Deglycosylation, IdeS Digestion, and Reduction;** Steve Murphy¹; Zach Van Den Heuvel¹; Maryann Shen²; Jing Chen¹; ¹Agilent Technologies, Inc., Madison, WI; ²Agilent Technologies, Santa Clara, CA
- WP 052 **Method Development of a Novel PK assay for Antibody-conjugated Drug Measurement of ADCs using Peptide-linker-drug Analyte;** Suk-Joon Hyung¹; Neelima Koppada¹; Surinder Kaur¹; Ola M Saad¹; ¹Genentech Inc, South San Francisco, CA
- WP 053 **Linker-Drug Site Influences Antibody-Conjugated Drug Pharmacokinetic Assay Development for Antibody-drug Conjugates (ADCs);** M. Violet Lee¹; Surinder Kaur²; Ola Saad²; ¹Genentech, South San Francisco, CA; ²Genentech Inc, South San Francisco, CA
- WP 054 **Fast Online Characterization of Cetuximab Fd-Glycoprotein by Direct Monitoring and Control of a Mammalian Cell Cultivation Using Ultrahigh-Resolution QTOF Analysis;** Martin Hedström¹; Constantin Issleib¹; Fredrik Olsson²; Dag Erlandsson¹; Anja Wiechmann³; Anja Resemann³; Catherine Evans⁴; Guillaume Tremintin⁵; Jason S. Wood⁶; Detlev Suckau³; Wolfgang Jabs³; ¹CapSenze HB, Lund, Sweden; ²Genovis AB, Lund, Sweden; ³Bruker Daltonik GmbH, Bremen, Germany; ⁴Bruker UK Ltd, Coventry, UK; ⁵Bruker, Fremont, CA; ⁶Bruker Daltonik, Billerica, MA
- WP 055 **Advancing Attribute Control of Antibodies Drug Conjugates (ADCs) using High Resolution Analytics;** Liuxi Chen¹; Henry Y Shion¹; Barbara Sullivan²; Ying-Qing Yu¹; Weibin Chen³; ¹Waters Corp., Milford, MA; ²Waters Corporation, Beverly, MA; ³Waters Corporation, Milford, MA
- WP 056 **Physicochemical Structural Characterization of Innovator and Biosimilar Eculizumab with High Resolution Mass Spectrometry Methods;** Maksim Degterev¹; Maksim Smolov¹; Grigoriy Poroshin¹; Rakhim Shukurov¹; ¹IBC Generium, Vol'ginskiy, Vladimirskaia Oblast'
- WP 057 **Probing Monoclonal Antibody-Protein Interactions by Native Mass Spectrometry on a Quadrupole Orbitrap Mass Spectrometer;** Hongxia (Jessica) Wang¹; Haibo Qiu¹; Jonathan L Josephs²; Eugen Damoc³; Ning Li¹; ¹Regeneron Pharmaceuticals, Tarrytown, NY; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Bremen, DE
- WP 058 **Top-down Characterization of Monoclonal Antibody on an Orbitrap Fusion Lumos Tribrid Mass Spectrometer;** Seema Sharma¹; Stephane Houel¹; Christopher Mullen¹; Chad Weisbrod¹; Romain Huguet¹; John Syka¹; David Horn¹; Jonathan Josephs¹; Jae Schwartz¹; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 059 **Complete Characterization of Biotherapeutic Proteins by Automated Data Processing on High Resolution Accurate Mass Spectrometry with SWATH® Acquisition;** Milla Neffling¹; Yang Shi¹; Dominic Gostick¹; Doug Simmons²; ¹SCIEX, Concord ON, Canada; ²SCIEX, Concord, ON
- WP 060 **Full Characterization of Heterogeneous Antibody Samples under Denaturing and Native/Native-Like Conditions on a Hybrid Quadrupole-Orbitrap Mass Spectrometer;** Kai Scheffler¹; Eugen Damoc²; Aaron Bailey³; Stephane Houel³; Jonathan L Josephs³; ¹Thermo Fisher Scientific, Dreieich, DE; ²Thermo Fisher Scientific, Bremen, DE; ³Thermo Fisher Scientific, San Jose, CA
- WP 061 **High Resolution Mass Spectrometry of a Bispecific Antibody for the Treatment of Pertussis;** Ellen K Wagner¹; Andre Bui¹; Tingting Wang¹; Maria D Person¹; Jennifer A Maynard¹; ¹University of Texas at Austin, Austin, TX

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- WP 062 **Serum Haptoglobin Glycosylation as a Potential Biomarker to Monitor Lung Cancer Development;** Ruiqing Zhang¹; Yujie Liu¹; Dan Zhang¹; Zhili Li²; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; ²IBMS, CAMS&PUMC, Beijing
- WP 063 **Urine Peptidome Study as a Promising Approach for Preeclampsia Diagnosis;** Natalia Starodubtseva^{1,2}; Alexey S Kononikhin^{1,2}; Anna Bugrova^{1,3}; Igor A Popov^{1,2,3}; Victoria Shirokova^{2,4}; Maria Indeykina^{3,4}; Olga Vavina¹; Kamila Muminova¹; Yuriy Kostyukovich^{2,5}; Vitaliy Chagovets¹; Vadim Lagutin¹; Evgeny Kukaev^{2,3}; Vladimir E Frankevich¹; Zulfia Khodzhaeva¹; Gennady Sukhikh¹; Eugene Nikolaev⁴; ¹Research Center for Obstetrics and Gynecology, Moscow, Russia; ²Moscow Institute of Physics and Technology, Moscow, Russia; ³Emanuel Institute of Biochemical Physics, Moscow, Russia; ⁴Institute for Energy Problems of Chemical Physics, Moscow, Russia; ⁵Skolkovo Institute of Technology, Moscow, Russia
- WP 064 **Identification of Serum Protein Biomarkers Associated with Early Heterotopic Ossification Formation following Traumatic Injury;** Michael E. Hoover¹; Claire Llamas²; Elizabeth C. Martin²; Elaine Boos³; Peter C. Krause³; Andrew G. King³; Harry Molligan³; Olivia C. Lee³; Vinod Dasa³; Thomas A. Davis⁴; Ammar Qureshi⁴; Benjamin Levi⁵; Jonathan A. Forsberg⁴; Jeffrey M. Gimble²; Michael A. Freitas¹; ¹Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH; ²Center for Stem Cell Research and Regenerative Medicine, Tulane University, New Orleans, LA; ³Department of Orthopedics, LSU Health Sciences Center, New Orleans, LA; ⁴Department of Regenerative Medicine, Naval Medical Research Center, Silver Spring, MD; ⁵Department of Surgery, University of Michigan, Ann Arbor, MI
- WP 065 **Identification of Nephropathy Prognostic Markers in Urine from Children Affected by type-1 Diabetes;** Magagnotti Cinzia¹; Gianpaolo Zerbini¹; Isabella Fermo¹; Rose Mary Carletti^{2,3}; Riccardo Bonfanti¹; Fabiana Vallone¹;

- WP 066 Arianna Restivo⁴; Giambattista Capasso⁴; Annapaola Andolfo¹; ¹OSR, Milan, Italy; ²IEO, Milan, Italy; ³IFOM, Milan, Italy; ⁴Second University of Naples, Naples, Italy
Deep Profiling of Extracellular Vesicles in μ L-Scale Plasma Samples Using Miniaturized Isolation Combined with Advanced Separation and MS Data Acquisition; Simion Kreimer¹; Arseniy M Belov¹; Rosa I Viner²; Marcia Santos³; Barry L Karger¹; Alexander R. Ivanov¹; ¹Northeastern University, Boston, MA; ²Thermo Fisher Scientific, San Jose, CA; ³SCIEX, Redwood City, CA
- WP 067 **Selection of Protein Biomarkers in Dehalococcoides Mccartystrains Enables an MRM-MS Approach for Monitoring Dechlorination Activities in Environmental Samples;** Manuel Villalobos^{1,2}; Karuna Chourey²; Frank Loeffler¹; Robert Hettich^{1,2}; ¹University of Tennessee-Knoxville, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- WP 068 **Proteomic Analysis of Plasma Extracellular Vesicles and the Impact of Sampling Conditions;** Ole Østergaard¹; Julia Tanas Tanassi²; Henrik Niels Helweg Heegaard¹; ¹Statens Serum Institut, Copenhagen, Europe; ²Statens Serum Institut, Copenhagen, Denmark
- WP 069 **Methodological Development for Exosome Enrichment in Serum;** Yan Ren¹; Jin Zi¹; Liang Lin¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China
- WP 070 **Serum N-glycome Analysis of Colorectal Cancer Patients Reveals Association with Survival;** Stefan W de Vroome¹; Stephanie Holst¹; Mar DM Rodriguez Girondo¹; Bart JA Mertens¹; Yuri EM van der Burgt¹; Wilma E Mesker¹; Manfred Wuhler¹; Rob AEM Tollenaar¹; ¹Leiden University Medical Center (LUMC), Leiden, The Netherlands
- WP 071 **Identification of Urinary Protein Biomarkers for Diagnosis of Hepatocellular Carcinoma by an Onco-proteogenomics Approach;** Thomas S.-H. Chiou^{1,2}; Chun-Hao Huang^{1,3}; Shu-Wen Chi¹; Chao-Jen Kuo¹; King-Teh Lee¹; ¹Kaohsiung Medical University, Kaohsiung, Taiwan; ²Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; ³Weill Graduate School of Medicine, Cornell University, Ithaca, NY
- WP 072 **The Ascites N-glycome of Epithelial Ovarian Cancer Patients;** Karina Biskup^{1,2}; Elena I Braicu³; Jalid Sehoul³; Rudolf Tauber¹; Véronique Blanchard¹; ¹Institute of Laboratory Medicine, Clinical Chemistry and Pathobiochemistry, Charité Medical University, Berlin, Germany; ²Department of Biology, Chemistry and Pharmacy, Freie University of Berlin, Berlin, Germany; ³Department of Gynecology, Berlin, Germany
- WP 073 **Blood Proteins with Isoelectric Point Close to 7.4 as Alzheimer Disease Biomarker;** Mohammad Pirmoradian Najafabadi^{1,2}; Thorleif Lavold²; Dag Aarsland^{3,4}; Roman A Zubarev¹; ¹Karolinska Institutet, Solna, Sweden; ²Biomotif AB, Stockholm, Sweden; ³Karolinska Institutet, Stockholm, Sweden; ⁴King's College London, London, UK
- WP 074 **Searching for CSF Biomarkers in PGRN Associated Frontotemporal Dementia;** Diana Nijholt¹; Lieke Meeter¹; Christoph Stingl¹; Lennard Dekker¹; Jeroen van Rooij¹; Shami Melhem¹; Theo M. Luider¹; John van Swieten¹; ¹Erasmus Medical Center, Rotterdam, The Netherlands
- WP 075 **Expanding the CSF Endopeptidome by High-pH reversed-phase Fractionation and LC-MS/MS;** Karl Hansson¹; Elin Pernevik¹; Silke Kern¹; Kaj Blennow¹; Henrik Zetterberg¹; Johan Gobom¹; ¹Gothenburg University; Institute of Neuroscience and Physiology, Gothenburg, Sweden
- WP 076 **Clinical CSF Proteomics and Endopeptidomics for Biomarker Identification in Neurodegenerative Diseases;** Johan Gobom¹; Karl Hansson¹; Elin Pernevik¹; Tobias Skillback¹; Henrik Zetterberg¹; Kaj Blennow¹; ¹University of Gothenburg, Institute of Neuroscience and Physiology, Gothenburg, Sweden
- WP 077 **Identifying Prostate Cancer Biomarkers by Profiling Glycoproteins in Human Prostate Tissue;** David Spiciarich¹; Sophia L. Maund²; Sean Purcell³; Anthony T Iavarone³; Donna M. Peehl²; Carolyn R Bertozzi^{4,5}; ¹University of California, Berkeley, CA; ²Stanford University School of Medicine, Palo Alto CA, USA; ³UC Berkeley, Berkeley, California; ⁴Stanford University, Stanford, CA; ⁵Howard Hughes Medical Institute, Chevy Chase, MD
- WP 078 **Mass Spectrometry-Based Proteomics of Human Breast Milk to Assess Breast Cancer Risk Using Different Protein Digestion procedures;** Roshanak Aslebagh¹; Kathleen F Arcaro²; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²University of Massachusetts Amherst, Amherst, MA
- WP 079 **Mass Spectrometric Analysis of Salivary Proteins from Medical Residents Performing Advanced Clinical Simulations Resulting in Acute Stress;** Rachel Marvin¹; Muncharie Brooke Saepoo¹; Paul Rega¹; Viviane Kazan¹; Kenneth Hensley¹; David Giovannucci¹; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH
- WP 080 **High Through-Put Quantitative Proteomics for the Discovery of Circulating Biomarkers in Cancer;** Hong Wang¹; Juan Chen¹; Xiaolian Liu¹; Clemente Aguilar Bonavides¹; Amin Momin¹; Hiroyuki Katayama¹; Sam Hanash¹; ¹MD Anderson Cancer Center, Houston, TX
- WP 081 **Proteomic Approach towards Early Diagnosis of Ventilator-Associated Pneumonia (VAP) in Critically Ill Patients;** Khyatiben Pathak¹; Marissa Saltzman²; Emmanuel B Menashi³; Frederic Zenhausem⁴; Patrick Pirrotte²; ¹Center for Proteomics, The Translational Genomics Research Institute, Phoenix, AZ; ²Center for Proteomics, Translational Genomics Research Institute, Phoenix, AZ; ³Laboratory for Genomics and Personalized Medicine, Honor Health Research Institute, Scottsdale, AZ; ⁴Center for Applied Nanobioscience and Medicine, University of Arizona, Phoenix, AZ
- WP 082 **Intact Protein Profiling of Proteoforms Moves toward the Clinic: Intact Protein Classification of Patients with Acute Rheumatic Fever;** Giuseppe Infusini¹; Laura Dagley²; Willy-John Martin²; Liam O'Connor²; Ian Wicks²; Andrew Webb²; ¹Walter & Eliza Hall Institute, Parkville, VIC; ²Walter & Eliza Hall Institute, Parkville, Australia
- WP 083 **A SWATH-MS Method to Monitoring Oxidative Stress and Progression to Cell Death: From Secretome to Blood Diagnosis;** Sandra Anjo¹; Vera Mendes¹; Mário Grãos^{1,2}; Bruno Manadas¹; ¹Center for Neurosciences and Cell Biology, Coimbra, Portugal; ²Biocant - Biotechnology Innovation Center, Cantanhede, Portugal
- WP 084 **Chronic Human African Trypanosomiasis Biomarker Discovery Using Quantitative Proteomics;** Matthew Szucs¹; Rushdy Ahmad¹; Brett Eyford²; Terry Pearson²; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²University of Victoria, Victoria BC, Canada
- WP 085 **Application of Adductomics for Investigating Biomarkers Associated with Ovarian Cancer;** Daniel Lador¹; William Funk²; ¹Northwestern University, Chicago, IL; ²Northwestern University, Evanston, IL
- WP 086 **Serialized Nanoparticle-Mediated Enrichment and Profiling of the Saliva Proteome;** Marissa Saltzman¹; Kelsey Mitchell²; Kristine Tsantilas¹; Khyati Pathak¹; Christophe Legendre¹; Victoria David¹; Matthew Rosenow¹; Shane Caswell³; Lance Liotta²; Emanuel Petricoin²; Patrick Pirrotte¹; ¹Translational Genomics Research Institute, Phoenix, AZ; ²Center for Applied Proteomics and Molecular Medicine, Manassas, VA; ³Sports Medicine Assessment Research and Testing (S.M.A.R.T.) Laboratory, Manassas, VA

- WP 087 **Identification of Serum Biomarker Candidates for Fatty Liver Disease through Depletion of Common High-Molecular-Weight Proteins;** Sachin Sridharan¹; Sobanaa Jayakumar¹; Keerthana Vinodh¹; Adaikkalam Vellaichamy¹; ¹Anna University, Chennai, India
- WP 088 **Analysis of Possible Biomarkers for Complex Regional Pain Syndrome and Osteoporosis using nLC-MS;** Johan Jacksén¹; Linus Svenberg¹; Åsa Emmer¹; ¹KTH Royal Institute of Technology, Stockholm, Sweden
- BIOMARKERS: QUANTITATIVE ANALYSIS (PART 2)**
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- WP 089 **Targeted Quantification of Mutant SPOP Proteins in Prostate Cancer;** Hui Wang¹; Christopher E. Barbieri²; Jintang He¹; Yuqian Gao¹; Chaochao Wu¹; Athena A. Schepmoes¹; Thomas L. Fillmore¹; Tujin Shi¹; Sung-Suk Chae²; Dennis Huang²; Juan Miguel Mosquera²; Wei-Jun Qian¹; Richard D. Smith¹; Sudhir Srivastava³; Jacob Kagan³; David Camp¹; Karin D Rodland¹; Mark A. Rubin²; Tao Liu¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Institute of Precision Medicine of Weill Cornell Medical College and New York Presbyterian Hospital, New York, NY; ³National Cancer Institute, Bethesda, MD
- WP 090 **Quantitative Tau Isoform Differentiation;** Paul Auger¹; Stephen Schauer²; W. Rodney Mathews¹; Lee Honigberg¹; Kristin R Wildsmith¹; ¹Genentech, South San Francisco, CA; ²Genentech Inc, South San Francisco, CA
- WP 091 **Developing LC-MS Assay for Pituitary Adenylate Cyclase-Activating Polypeptide;** Ruina Li¹; Yuzhong Deng¹; Brian Dean¹; Xiaorong Liang¹; ¹Genentech Inc, South San Francisco, CA
- WP 092 **Proteomic and Biochemical Analyses of EAM Rat;** Jong Bok Seo¹; Soo Jeong Park¹; Seung Min Choi²; ¹Korea Basic Science Institute, Seoul, Republic of Korea; ²Korea Basic Science Institute, Seoul, Republic of Korea
- WP 093 **Development of a Sensitive LC-MS/MS Method to Quantify Substance P Concentrations in Rat Cerebrospinal Fluid;** Hanumanth Rao Pantangi¹; Lakshmi Prasanna Rayapati¹; Prathyusha Chunduru¹; Saivishal Daripelli¹; Ganesh Ayyanki¹; Venkatesh Kamuju¹; Ramakrishna Nirogi¹; ¹Suven Life Sciences Ltd, Hyderabad, Telangana
- WP 094 **MRM-based Assay for Potential Protein Biomarker in Meningioma Patients;** Shuvolina Mukherjee¹; Ajit Datar²; Rashi Kochhar²; Sanjeeva Srivastava¹; Vedita Anand Singh¹; Nikita Gahoi¹; Saicharan Ghantasala¹; Aliasgar Moiyadi³; Epari Sridhar³; ¹Indian Institute of Technology Bombay, Mumbai, INDIA; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA; ³Tata Memorial Center, Mumbai, INDIA
- WP 095 **MRM Based Targeted Analysis of Serum Samples to Demonstrate Differentially Expressed Proteins in Severe Cases Of Falciparum Malaria;** Vipin Kumar¹; Shailesh Damale²; Ajit Datar²; Sanjeeva Srivastava¹; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- WP 096 **Development of MRM Assay for the Determination of Potential Biomarkers in Case of Severe Vivax Malaria;** Sandip Patel¹; Shailendra Rane²; Ajit Datar²; Swati Patankar¹; Sanjeeva Srivastava¹; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- WP 097 **Quantitative Profiling of Hypoxia-responsive Cellular Pathways Associated with Metastasis in Osteosarcoma by Parallel Reaction Monitoring Assay;** Zifeng Song¹; Liping Yang¹; Luisa Zini²; Caleb Emmons²; Siva Kolluri¹; Millan Shay¹; Milan Milovancev¹; Claudia S Maier¹; ¹Oregon State University, Corvallis, OR; ²Proteome Software, Portland, OR
- WP 098 **Analysis of Glycosylation of Serum CD90 in Pancreatic Cancer by Mass Spectrometry;** Jun Cao^{1,2}; Jianhui Zhu¹; Rui Yang¹; Zhijing Tan¹; Mingrui An¹; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²Hangzhou Normal University, Hangzhou, China
- WP 099 **Quantification of the Unique eEF2 His715-Diphthamide post-translational Modification and Its Derivatives by Parallel Reaction Monitoring Mass Spectrometry;** Axel Ducret¹; Sabine Kux van Geijtenbeek¹; Sebastian Stahl²; Ana Rita da Silva Mateus Seidl²; Sven Michel²; Gerhard Niederfellner²; Ruediger Rueger²; Ulrich Brinkmann²; ¹F. Hoffmann-La Roche Ltd, Basel, Switzerland; ²F. Hoffmann-La Roche Ltd, Penzberg, Germany
- WP 100 **Analysis of Human Dried Blood Spots for Cotinine and trans-3'-Hydroxycotinine by Reversed Phase Ultra Performance Liquid Chromatography Tandem Mass Spectrometry;** Alexandria L Anstett^{1,2}; Michael C. Stagliano²; S. Alexandra Burt¹; Matthew J Geiger²; Sara E Tomechko²; ¹Michigan State University, East Lansing, MI; ²MI Department of Health & Human Services, Lansing, MI
- WP 101 **Novel Proteomics-Based Pipeline for Identifying Predictive Biomarkers of Taxane-Induced Neuropathy;** Emily Chen¹; Katherine D. Crew^{2,3}; Meghna Trivedi²; Danielle Awad⁴; Mathew Maurer²; Kevin Kalinsky^{2,4}; Antonius Koller⁵; Purvi Patel⁵; Jenny Kim Kim⁵; Dawn Herschman^{2,3,4}; ¹Columbia University Medical Center, New York, NY; ²Department of Medicine, Columbia University Medical Center, New York, NY; ³Department of Epidemiology, Columbia University Medical Center, New York, NY; ⁴Herbert Irving Comprehensive Cancer Center, New York, NY; ⁵Herbert Irving Comprehensive Cancer Center, Proteomics Shared Resource, New York, NY
- WP 102 **Quantification of Lysosomal Storage Disease Specific Urinary Oligosaccharides for Potential Treatment Monitoring;** Rongrong Huang¹; Allison Cason¹; Laura Pollard¹; Tim Wood¹; ¹Greenwood Genetic Center, Greenwood, SC
- WP 103 **Evaluation of Stable Isotope Dimethyl Labeling and Spectra Counting for Protein Profiling in Mice with Nonalcoholic Steatohepatitis;** Zhicheng Jin¹; Takhar Kasumov²; ¹Northeast Ohio Medical University, Rootstown, OH; ²Northeast Ohio Medical University, Rootstown, OH
- WP 104 **Rapid Detection of a Low-Abundance Biomarker from Plasma Using Combined Capture and Digestion for Improved Sensitivity;** John O'Grady¹; Kevin Meyer¹; Derrick Poe¹; ¹Perfinity Biosciences, Inc West Lafayette, IN
- WP 105 **Multiplexed Longitudinal Monitoring of Cancer Biomarkers in Dried Blood Spots using an Automated SISCAPA Workflow;** Morteza Razavi¹; Leigh Anderson¹; Richard Yip¹; Matthew E. Pope¹; Terry W Pearson¹; ¹SISCAPA Assay Technologies, Washington, DC
- WP 106 **Standardizing Targeted Mass Spectrometry Quantification of Dystrophin Toward Implementation in Clinical Trials;** Kristy J Brown¹; Meng Hsuan Han¹; Mamta Giri¹; Shivaprasad Bhuvanendran¹; Jyoti Jaiswal²; Eric P Hoffman¹; Yetrib Hathout¹; ¹Children's National Healthy System, Washington DC, DC; ²Children's National Medical Center, Washington, DC
- WP 107 **Rapid QQQ Screening and Quantification of Proteins from Complex Biological Matrices using Retention Time Predictor without Expensive Protein Standards;** Rohana Liyanage¹; Balamurugan Packialakshmi²; Jeremy Post³; Narayan C. Rath⁴; Jackson O. Lay, Jr²; ¹University of Arkansas, Fayetteville, AR; ²University of Arkansas, Fayetteville, AR; ³Shimadzu Scientific Instruments, Columbia, MD - Maryland; ⁴PPPSRU, USDA, Agricultural Research Service, Fayetteville, AR

- WP 108 **Development of Peripheral Blood Mononuclear Cell (PBMC) Based Protein Biomarkers for Lung Cancer Diagnosis using DIA Mass Spectrometry**; Shaohua Xu¹; Chunlin Cai²; Feng Yao³; Qian Wu⁴; Heng Zhao³; Wei Yan²; ¹Shanghai Jiatong University, Shanghai, China; ²Shanghai Jiao Tong University, Shanghai, China; ³Shanghai Chest Hospital, Shanghai, China; ⁴Shanghai Center for Bioinformation Technology, Shanghai, China
- WP 109 **High Sensitivity and High Specificity LC-HRMS Method to Quantify the Corticosteroid Metabolome after Exposure to Inhaled Corticosteroids**; Clementina A. Mesaros¹; Dominic Ciccimaro^{1,2}; Nathaniel W Snyder³; Ian A Blair^{1,2}; ¹University of Pennsylvania, Philadelphia, PA; ²Penn SRP Center and CEET, Philadelphia, PA; ³AJ Drexel Autism Institute, Philadelphia, PA
- WP 110 **Quantitative Evaluation towards the Glutathione S-Transferases in Human Plasma Using Affinity Coupling with LC-MS/MS**; Feng Xian; Beijing Institute of Genomics, CAS, Beijing, Beijing
- WP 111 **Absolute Quantitation of Biomarkers Predictive of Recovery from Acute Kidney Injury after Liver Transplantation with nano-LC - Triple-Quad Mass Spectrometry**; Jacek W Sikora¹; Paul M Thomas²; Joshua Levitsky^{3,4}; Neil L Kelleher²; ¹Proteomics Center of Excellence, Northwestern University, Evanston, IL; ²Proteomics Center of Excellence, Northwestern University, Evanston, IL; ³Comprehensive Transplant Center, Northwestern University Feinberg School of Medicine, Chicago, IL; ⁴Division of Gastroenterology and Hepatology, Northwestern University Feinberg School of Medicine, Chicago, IL
- WP 112 **Towards Routine Sub 100uL Serum/Plasma Analysis of Hepcidin-25 using LC/MS/MS**; Joel Gummer^{1,2,3}; Ben Hunter^{1,2}; Robert Trengove^{2,3,4}; ¹School of Veterinary and Life Sciences, Murdoch University, Perth, Australia; ²Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; ³Metabolomics Australia, WA Node, Perth, Australia; ⁴Murdoch University, Murdoch, WA
- WP 113 **Simultaneous Determination of Ceftazidime and Avibactam in Human Plasma by LC/MS**; Xiaohua Li¹; Xu Allan¹; ¹Keystone Bioanalytical, Inc. North Wales, PA
- WP 114 **Integrating Glycoproteomics in the Comprehensive Multi-Omics Profiling of Obesity-mediated Progression to Type II Diabetes**; Christine Yeh; Stanford, California
- WP 115 **An ABRF-PRG study: Identification of Low Abundance Proteins in a Highly Complex Protein Sample**; Susan Van Riper¹; Chen Emily²; Allis Chien³; Henriette Remmer⁴; Paul M. Stemmer⁵; Wang Yan⁶; Pratik Jagtap⁷; ¹University of Minnesota Informatics Institute, University of Minnesota, Minneapolis, MN; ²Herbert Irving Comprehensive Cancer Center & Department of Pharmacology, Columbia University Medical Center, New York, NY; ³Stanford University Mass Spectrometry, Stanford University, Stanford, CA; ⁴Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; ⁵Institute of Environmental Health Science, Wayne State University, Detroit, MI; ⁶Proteomics Core Facility, University of Maryland, College Park, MD; ⁷Center for Mass Spectrometry and Proteomics, University of Minnesota, St. Paul, MN
- WP 116 **Particle-based N-linked Glycan Analysis of Selected Serum Proteins using Non-Glycosylated Binders as a Cancer Array Assay**; Isabella Karlsson¹; Anna Sroka-Bartnicka¹; Alessandro Quaranta¹; Lorena Ndreu¹; Matthijs Pijnappel¹; Gunnar Thorsén¹; ¹Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden
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- WP 119 **In-depth Analysis of Non-derivatized N-linked Glycans Using Ion Chromatography- Orbitrap Mass Spectrometry**; Zoltan Szabo¹; Junhua Wang²; Yury Agroskin¹; Rosa Viner³; Julian Saba³; ¹Thermo Fisher Scientific Japan, Yokohama, Japan; ²Thermo Fisher Scientific Inc, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA
- WP 120 **Hydrophilic Interaction Liquid Chromatography-Mass Spectrometric Imaging Platform for N-glycan Relative Quantitation using Stable-Isotope Labeled Hydrazide Reagents**; Zhengwei Chen¹; Xuefei Zhong²; Tie Cai³; Yatao Shi²; Xinxiang Zhang⁴; Lingjun Li²; ¹University of Wisconsin Madison, Madison, WI; ²University of Wisconsin-Madison, Madison, US; ³Peking University, Beijing, China; ⁴Chinese Academy of Sciences, Shanghai, China
- WP 121 **A Comprehensive Mass Spectrometric Workflow to Investigate Glycosylation Impact on Viral Antigenic Sites**; Edward Bodnar¹; Lisa Parsons¹; Yanming An¹; John F Cipollo¹; ¹Human and Health Services, U.S. Food and Drug Administration, Division of Bacterial, Parasitic and Allergenic Products, Laboratory of Bacterial Polysaccharides, Silver Spring, USA
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- WP 124 **Speeding up the High Throughput Searches for Glycan Analysis**; Ningombam Sanjib Meitei¹; Arun Apte²; Rupanjana Goswami¹; Julian A Saba³; ¹PREMIER Biosoft, Indore, India; ²PREMIER Biosoft, Palo Alto, CA; ³Thermo Fisher Scientific, San Jose, CA
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- WP 126 **Multiplex LC-MS Analysis of Isotopically Permethylated N-glycans Derived From Biological Samples**; Xue Dong¹; Shiyue Zhou¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
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- WP 128 **Glyconote: A Software for the Automated Interpretation of Glycomics Data from Tandem Mass Spectrometry;** Mingqi Liu¹; Guy Treves²; Andres Guerrero²; Matthew Amicucci²; Jasmine Davis²; Lauren D Wu²; Pengyuan Yang¹; Carlito B Lebrilla²; ¹Fudan University, Shanghai, China; ²UC Davis Chemistry Department, Davis, CA
- WP 129 **Optimization of Dual Modifications Strategy for Simultaneous Characterization of Neutral and Sialylated N-Glycans by LC-MS/MS;** Haiying Li¹; Patricia Cho¹; Stephen Kostel¹; John Froehlich¹; Richard Lee¹; ¹Boston Children's Hospital, Harvard Medical School Boston, MA
- WP 130 **Semi-automated Glycan Screening and Quantitative Analysis of Longitudinal Plasma Samples;** Elizabeth S. Hecht¹; Alison Motsinger-Reif¹; Brendan MacLean²; James N Pettit¹; Michael J MacCoss²; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²University of Washington, Seattle, WA
- WP 131 **Sialyl Linkage-Specific Glycan Profiling using Solid-Phase SALSA: A Simple and Versatile Derivatization Approach;** Takashi Nishikaze¹; Hiroki Tsumoto²; Yuzo Yamazaki¹; Shinichi Iwamoto¹; Yuri Miura²; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Tokyo Metropolitan Institute of Gerontology, Tokyo, Japan
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- WP 134 **Glyc: A New Tool for Glycan Structure Elucidation and Characterization;** Eric Joyce¹; Jinshan Gao¹; ¹Montclair State University, Montclair, NJ
- WP 135 **Developmental Profiles of Gangliosides in Prefrontal Cortex of Human Brain via Negative Ion Mode Nano-LC/MS and LC/MS/MS;** Injung Ji^{1,2}; Jae Yun Hwang^{1,2}; Su Min Kim^{1,2}; Dan Bi Park^{1,2}; David Bradley³; Hyun Joo An^{1,2}; ¹Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea; ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea; ³Agilent technologies Inc, Santa Clara, CA
- WP 136 **Tailoring Glycan Hydrazide Tagging Reagents for MS Functionality;** James McCord¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, North Carolina
- WP 137 **Acid-Induced Fucose Migration;** Yi Pu¹; Yang Tang¹; John Haserick²; Catherine E Costello²; Cheng Lin²; ¹Boston University, Boston, MA; ²Boston University School of Medicine, Boston, MA
- WP 138 **Automated N-Glycan Sample Preparation with an Instant Glycan Labeling Dye for Mass Spectrometry;** Ted Haxo¹; Aled Jones; Michael J Kimzey¹; Emily Dale¹; Sergey vlasenko¹; Steve mast¹; ¹ProZyme, Hayward, CA
- WP 141 **Biomarkers of Early Chronic Obstructive Pulmonary Disease (COPD) in Smokers and Former Smokers - A Comparison of Two Methods;** Karin Barbara Sahlin¹; Johan Malm²; Mikael Truedsson^{2,3}; May Bugge³; Elisabet Wieslander²; Maria Yokaleva²; Magnus Dahlbäck²; Roger Appelqvist²; Thomas Fehniger²; György Marko-Varga²; ¹Lund University, Lund, Sweden; ²Lund University, Lund, Sweden; ³Örestadskliniken, Malmö, Sweden
- WP 142 **Large-Scale Analysis of Protein Conformational Changes for Biomarker Discovery;** Fang Liu¹; Michael C Fitzgerald¹; ¹Duke University, Durham, NC
- WP 143 **Study of Traumatic Brain Injury Biomarkers by Mass Spectrometry-Based Proteomics;** Manasi Mangaonkar¹; Richard A Yost¹; Kari Green¹; Kevin Wang¹; ¹University of Florida, Gainesville, FL
- WP 144 **Lipidomics Approach in Biliary Atresia for a Potential Diagnostic Method Based on Mass Spectrometry;** Cibele Esteves¹; Diogo Noin de Oliveira¹; Carlos Fernando Odor Rodrigues Melo¹; Luciana Di Paolo¹; Gabriel Hessel¹; Rodrigo Ramos Catharino¹; ¹University of Campinas, Campinas, Brazil
- WP 145 **Neonatal Neurodegeneration in 5XFAD Alzheimer's Disease Transgenic Mouse Model;** Aise Rumeysa Mazi^{1,2}; Aysegül Sumeyye Arzumani^{1,2}; Mehmet Ozansoy^{1,3}; Ahmet Tarik Baykal⁴; ¹Regenerative and Restorative Medicine Research Center, REMER, Istanbul, Turkey; ²Institute of Health Science, Istanbul Medipol University, Istanbul, Turkey; ³Department of Physiology, International School of Medicine, Istanbul Medipol University, Istanbul, Turkey; ⁴Acibadem University, Ataşehir-Istanbul
- WP 146 **A Proteomic Investigation of the Role of Neurotoxins Linked to Amyotrophic Lateral Sclerosis Disease Pathogenesis;** Joshua Beri¹; Michael S Bereman¹; ¹NC State University, Raleigh, NC
- WP 147 **Prediction of Response to Sorafenib in Hepatocellular Carcinoma: A Multimarker Panel of Potential Biomarkers by Multiple Reaction Monitoring-Mass Spectrometry;** Hyunsoo Kim¹; Injoon Yeo¹; Su Jong Yu²; Taesung Park³; Jung-Hwan Yoon²; Youngsoo Kim¹; ¹Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; ²Department of Internal Medicine and Liver Research Institute, Seoul National University College of Medicine, Seoul National University Hospital, Seoul, Korea; ³Department of Statistics, Seoul National University, Seoul, Korea
- WP 148 **Simultaneous Quantification of Tryptophan-Related metabolites as Biomarkers for Prediabetes;** Norihide Yokoi¹; Ritsuko Hoshikawa¹; Toshiya Matsubara²; Susumu Seino¹; ¹Kobe University Graduate School of Medicine, Kobe, JPN; ²SHIMADZU Corporation, Kyoto, JPN
- WP 149 **Comparison of Plasma Protein Profiles of Selected Cardiovascular Diseases by iTRAQ Quantification;** Helena Rehulkova¹; Alena Myslivcova Fucikova¹; Pavel Rehulka¹; Radek Pudil²; Jiri Stulik¹; ¹Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech Republic; ²1st Department of Internal Medicine – Cardioangiology, Faculty Hospital, Hradec Kralove, Czech Republic
- WP 150 **Proteomics Analysis of Aged Healthy Human White Blood Cells;** Ceereena Ubaida-Mohien¹; Alexey Lyashkov¹; Arsun Bektas¹; Robert Wersto¹; Nan Ping Weng¹; Ranjan Sen^{1,2}; Luigi Ferrucci¹; ¹Intramural Research Program, National Institute on Aging, National Institutes of Health, Baltimore, MD - Maryland; ²Laboratory of Molecular Biology and Immunology, National Institute on Aging, Baltimore, MD
- WP 151 **Cardiovascular Disease - Metabolic Syndrome Induced Protein/PTM Changes;** Mark E. McComb¹; Stephen A. A Whelan¹; Chunxiang Yao¹; Jessica B. Behring¹; Jean L. Spencer¹; Christian F. Heckendorf¹; Nancy M. Leymarie¹;

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- WP 140 **Identification of a CNS-specific Proteome Biomarker for Clinical Relapses and Progression of Multiple Sclerosis using a Systems-Biology Approach;** Itay Raphael¹; Carol A Huizar¹; Yanyan Qu²; Wendell P Griffith²; Thomas G Forsthuber¹; ¹Department of Biology, University of Texas at San Antonio, San Antonio, TX; ²Department of Chemistry, University of Texas at San Antonio, San Antonio, TX

Deborah A. Siwik¹; Wilson S. Colucci¹; Richard A. Cohen¹; Markus M. Bachschmid¹; Catherine E. Costello¹; ¹*Boston University School of Medicine, Boston, MA*

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WP 163 **Evaluation of Ion Mobility Enabled Collisional Cross Section Measurements for the Differentiation of Acyl and Phenolic Glucuronide Metabolites**; Catherine Holdsworth¹; Richard Clayton¹; Daniel Weston²; Nick Tomczyk²; Martin Palmer²; Darren Hewitt²; ¹*Covance, Harrogate, UK*; ²*Waters, Wilmslow, UK*

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WP 165 **Automatic Calculation and Layout of MS/MS Fragmentation Pathways**; Ismael Zamora¹; Blanca Serra²; Moretoni Luca³; ¹*Lead Molecular Design, S.L., Sant Cugat del Valles, Barcelona*; ²*Molecular Discovery, Ltd London, UK*; ³*Molecular Discovery, London, UK*

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WP 169 **Rapid Rank Ordering of Compounds in Mixtures by Orthogonal Affinity Selection – Mass Spectrometry**; Christine L. Andrews¹; Matthew P Richards¹; Jacqueline Hicks¹; John Caldwell¹; Jared Cumming¹; Andrew Stamford¹; Corey Strickland¹; Peter Dandliker¹; ¹*Merck & Co, Kenilworth, NJ*

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- WP 178 **Detection of Creatine from Single Algae Cells using Mass Spectrometry;** Mei Sun¹; Ning Pan¹; Boris Wawrik¹; Zhibo Yang¹; ¹The University of Oklahoma, Norman, OK
- WP 179 **Quadrupole-Time-of-Flight Tandem Mass Spectrometry Identifies and Quantifies Eugenol in Extraction from Bio-oils Into Diesel;** Kelsey Boes¹; Nelson R Vinuesa¹; Yufei F Chen¹; Hoyong Kim¹; Park Sunkyu¹; ¹North Carolina State University, Raleigh, NC
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- WP 182 **Investigating the Mechanism of Lipid Body Obesity in *C. reinhardtii* under Nitrogen Starvation Conditions using High Resolution Mass Spectrometry;** Carter Lantz¹; Ryan Rho¹; Jeremy Sieker¹; Matthew Brantley¹; Alireza Abdolvahabi¹; James Chang¹; Sung-Joon Kim¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- WP 183 **Effect of Alkali Metals on Pyrolysis Kinetics of Carbohydrates Using dAPCI-TOF MS;** Kristen O'Connor¹; Carolyn Hutchinson¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- WP 184 **Characterization of Fast Pyrolysis Oil from Pine Feedstock;** Ashley Wittrig¹; Ross Mabon¹; Boris Sheludko¹; ¹ExxonMobil, Annandale, NJ
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- WP 187 **Integrated Omics Reveals the Details of Metabolic Adaptation of *Clostridium thermocellum* ATCC-27405 Grown on Switchgrass;** Suresh Poudel^{1,2}; Richard J Giannone¹; Miguel Rodriguez¹; Babu Raman³; Madhavi Z Martin¹; Nancy L Engle¹; Nookaew Intawat¹; Steven D Brown¹; Timothy J Tschaplinski¹; David Ussery¹; Hettich L Robert¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN; ³Dow AgroSciences, Indianapolis, IN
- WP 188 **Large scale Identification of Polymorphic Peptides via Cross-Species Spectral Networks in Microbial Proteomics;** Seungjin Na¹; Sam Payne²; Nuno Bandeira¹; ¹University of California San Diego, La Jolla, CA; ²Pacific Northwest National Lab, Richland, WA
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- WP 191 **Water Quality Growth and Change, Advanced Technology Method Change to Prescribe a Desirable Future to US EPA Method 521, (2004);** Andrew Eaton¹; Konjit Tadigo¹; Charles Grady¹; Ron Honnold²; ¹Eurofins Eaton Analytical Inc, Monrovia, CA; ²Agilent Technologies, Prescott, AZ
- WP 192 **A New Approach for Identification of Unknown Disinfection Byproducts in Drinking Water using Multiplex Solid Phase Extraction /HPLC-tandem Mass Spectrometry;** Xing-Fang Li¹; Yanan Tang²; Guang Huang²; Lindsay Jmaiff²; Ian Vander Meulen²; ¹University of Alberta, Edmonton, AB; ²University of Alberta, Edmonton, Canada
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- WP 194 **Significantly Improved Detection in Volatile Organic Analysis (VOA) of Water using Static Headspace and GCMS with a High Efficiency Source;** Harry Prest¹; Melissa Churley²; Peter Gautsch³; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies Sales & Services GmbH, Waldbronn, Deutschland
- WP 195 **Increased Capabilities for the Analysis of Hormones in Drinking and Waste Water using SPE and LC/MS/MS;** Xianrong (Jenny) Wei¹; Sean Orlovicz²; ¹Phenomenex, Torrance, ca; ²Phenomenex, Torrance, CA
- WP 196 **Analysis and "Fingerprinting" of Non-Ionic Surfactants in Hydraulic Fracturing Waters by Ion Mobility Mass Spectrometry;** E. Michael Thurman¹; Imma Ferrer²; Jerry Zweigenbaum³; Aaron Boice⁴; John Fjeldsted⁴; ¹University of Colorado, Boulder, CO; ²University of Colorado, Boulder, Colorado; ³Agilent Technologies, Little Falls, DE; ⁴Agilent Technologies, Santa Clara, CA
- WP 197 **Cloud-based Analysis of Complex Sample Systems for Outlier and Trend Analysis in the Context of Water Monitoring;** Ralf Tautenhahn¹; Tim J Stratton¹; Dipankar Ghosh¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 198 **Two Birds with One Stone: Simultaneous GC/MS Analysis of Volatile and Semivolatile Water Pollutants;** Olga V Polyakova¹; Dmitry Mazur¹; Viatcheslav Artaev²; Albert T. Lebedev³; ¹Moscow State University, Moscow, Russia; ²LECO Corporation, St Joseph, MI; ³Moscow State University, Moscow, Moscow
- WP 199 **Unknown Profiling of Drinking Water Using High Resolution LC-MS/MS and New Software;** Caroline DING¹; Anastasia Kalli¹; Charles Yang¹; Tim J Stratton¹; ¹Thermo Fisher Scientific, San Jose, CA
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- WP 289 **Trace Elemental Quantification of Carbon via the Production of Cyanide Anions in Plasma Assisted Reaction Chemical Ionization Mass Spectrometry (PARCI-MS);** Peter Haferl¹; Haopeng Wang¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC
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- WP 291 **Raising the Identification Confidence in Non-Target Analysis of House Dust by Combining Classic and Soft Electron Ionization GC-HRMS;** Peter Haglund¹; Sofia Nieto²; Vadim Kalmeyer²; Nathan Eno²; Jennifer Sanderson²; ¹Umea University, Umea; ²Agilent Technologies, Santa Clara, CA
- WP 292 **GCxGC with Simultaneous Mass Spectrometry/Flame Ionization Detection for Routine Petrochemical Analyses;** Laura McGregor¹; Nick P Bukowski¹; Matthew Edwards¹; Pete Grosshans²; Chris Hall²; Massimo Santoro¹; ¹Marks International, Cardiff, UK; ²Marks International Inc, Cincinnati, OH
- WP 293 **A High Efficiency Ion Source for GC/MS;** Jeffrey Kernan; ¹Agilent Technologies, Santa Clara, CA
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- WP 295 **Detailed Characterization of Glycans and Glycopeptides by Collisional and Electron Activated Dissociation;** Kshitij Khatri¹; Yi Pu¹; Joshua Klein¹; Cheng Lin¹; Joseph Zaia¹; ¹Boston University, Boston, MA
- WP 296 **Glycopeptide Analysis Using Parallel Data-Dependent Acquisition at Varied Normalized Collision Energies;** Crystal Daniels¹; Joseph Otto¹; Jana Rocker¹; Lindsay Schambeau¹; ¹Mitchell Cancer Institute, Mobile, AL
- WP 297 **Sequential Chemical Charge Enhancement with Electron-Transfer Dissociation for the Site-Specific Characterization of Doubly Glycosylated Peptides;** Yanyan Qu¹; William R Alley¹; Stephan Bach¹; Wendell P Griffith¹; ¹Department of Chemistry, University of Texas at San Antonio, San Antonio, TX
- WP 298 **Comparing Effectiveness and Specificity of Glycopeptide Enrichment Strategies for Qualitative LC-MS/MS Analysis of Depleted Human Plasma;** Sarah Michelle Totten¹; Majlinda Kullolli²; Christa Feasley³; Sharon J Pitteri²; ¹Stanford University School of Medicine, Palo Alto,

- CA; ²Stanford University School of Medicine, Palo Alto CA; ³Thermo Fisher Scientific, West Palm Beach, FL
- WP 299 **Online Cotton HILIC: An Easily Accessible and Affordable Enrichment of Glycopeptides;** Jingfu Zhao¹; Ehwang Song¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
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- WP 302 **N-glycosylation Analysis of Specific Serum Proteins using an Automated Microfluidic Platform and MALDI-MS;** Alessandro Quaranta¹; Anna Sroka-Bartnicka¹; Isabella Karlsson¹; Lorena Ndreu¹; Matthijs Pijnappel¹; Thorsén Gunnar¹; ¹Stockholm University, Stockholm
- WP 303 **Identification and Separation of N-glycans by HILIC/MS;** Zsuzsanna Lakos¹; Elena Dremena¹; Robert Carney¹; John L. Snyder¹; ¹Eurofins Lancaster Laboratories, Lancaster, PA
- WP 304 **Silk-Based Glyco-Enrichment Tip for Purification and Enrichment of Glycans and Glycopeptides;** Haci Mehmet Kayili^{1,2}; Mehmet Atakay¹; Bekir Salih¹; ¹Hacettepe University, Department of Chemistry, Ankara, Turkey; ²Çankırı Karatekin University, Department of Chemistry, Çankırı, Turkey
- WP 305 **N-linked Glycosylation Analysis of Seasonal Influenza Vaccine Hemagglutinins;** Yanming An¹; Lisa Parsons¹; John Cipollo¹; ¹FDA/CBER, Silver Spring, MD
- WP 306 **Assisting the Identification of Isomeric Glycoforms with a Hydrophilic Interaction Liquid Chromatography Retention Time Model for Procainamide Tagged N-linked Glycans;** Emily Betchy¹; Barry Boyes²; Ron Orlando¹; ¹CCRC, University of Georgia Athens, GA; ²Advanced Materials Technology, Wilmington, DE
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- WP 308 **Automated Processing of LC-MS/MS Data for Quantitative Analysis of the Human-like N-glycosylation of Glycoproteins Produced by a Glyco-optimization Cell Platform;** Robert Wilmanowski¹; Catherine Evans²; Anja Resemann³; Peter Hufnagel³; Rainer Paape³; Detlev Suckau³; Wolfgang Jabs³; Sven Bahrke¹; Keven Lothert¹; Andrea Hahne¹; ¹Glycotope GmbH, Berlin, Germany; ²Bruker Ltd, Coventry, UK; ³Bruker Daltonik GmbH, Bremen, Germany
- WP 309 **N-glycan Analysis using GIG-automation on Sialylglycotransferase Knock-in CHO Cell Line;** Shuang Yang¹; Qiong Wang²; Lijun Chen³; Bojiao Yin²; Li Shuwei⁴; Michael Betenbaugh²; Hui Zhang³; ¹John Hopinks Dept. of Pathology, Baltimore, MD; ²Johns Hopkins University, Baltimore, MD; ³Johns Hopkins School of Medicine, Baltimore, MD; ⁴University of Maryland, College Park, MD
- WP 310 **GPQuest: A Free Software for Identification of Glycans and Intact Glycopeptides;** Yingwei Hu¹; Shadi Toghi Eshghi²; Weiming Yang¹; Punit Shah¹; Shisheng Sun¹; Shuang Yang¹; Lingquan Deng¹; Xingde Li²; Hui Zhang¹; ¹Department of Pathology, School of Medicine, Johns Hopkins University, Baltimore, MD; ²Department of Biomedical Engineering, School of Medicine, Johns Hopkins University, Baltimore, MD
- WP 311 **Scalable Computational Tool for Identifying Intact Glycopeptides in Complex Samples Using Mass Spectrometry;** Lei Wang¹; Chuan-Yih Yu¹; Anoop M Mayampurath²; Rui Zhu³; Ehwang Song³; Yehia Mechref³; Haixu Tang¹; ¹Indiana University, Bloomington, IN; ²University of Chicago, Chicago, IL; ³Texas Tech University, Lubbock, Texas
- WP 312 **GLYMPs: A Tool to Automatically Assign Glycopeptides from MS/MS Data;** Lisa Parsons¹; Yanming An¹; John F Cipollo¹; ¹FDA/CBER, Silver Spring, MD
- WP 313 **Confident, Automated N-glycoproteomics Profiling in Unenriched and Glycopeptide-Enriched Cancer Cell Samples;** Shadab Ahmad¹; Amol Prakash¹; Sergei I Snovida²; Scott M Peterman³; Chu-Wei Kuo⁴; Kay-Hooi Khoo⁴; Gauri Muradia⁵; Jeremy P Kunkel⁵; Jessie R Lavoie⁵; Nina Soltero²; Julian A Saba²; ¹Optys Tech Corporation, Brighton, MA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Scientific BRIMS, Cambridge, MA; ⁴Academia Sinica, Taipei, Taiwan; ⁵Health Canada, Ottawa, Canada
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- WP 315 **MALDI Compatible Protease Chips - A Novel Platform For Protein H/D Exchange;** Michal Rosulek^{1,2}; Petra Darebna^{1,2}; Daniel Kavan^{1,2}; Petr Man^{1,2}; Michael Volny³; Petr Pompach^{1,2}; Petr Novak^{1,2}; ¹Institute of Microbiology CAS, Prague, Czech Republic; ²Faculty of Science, Charles University in Prague, Prague, Czech Republic; ³Affipro, s.r.o., Mratin, Czech Republic
- WP 316 **Protease Type XVIII Columns for Enhanced Digestion Efficiency and Sequence Resolution for Protein HDX Monitored by Q Exactive MS;** Chengjie Ji¹; Qian Li¹; Yankun Li¹; ¹Novabioassays LLC, Woburn, MA
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- WP 318 **In-source Column Cooling for nanoHX-MS on Complex Druggable Protein Scaffolds;** Joey Sheff¹; David Schriemer¹; ¹University of Calgary, Calgary, Canada
- WP 319 **Post-column Hydrogen-deuterium Exchange Method for the Identification of Organic Compounds;** Emmanuel Eysserie¹; Xavier Bellerose¹; Jean-Michel Lavoie¹; Pedro A Segura¹; ¹Université de Sherbrooke, Sherbrooke, QC
- WP 320 **How Precise are HDX-MS Measurements? Results from the NIST HDX-MS Interlaboratory Comparison Project;** Jeffrey W. Hudgens^{1,2}; Elyssia S Gallagher^{1,2}; Ioannis Karageorgos^{1,2}; ¹National Institute of Standards and Technology, Rockville, MD; ²Institute for Bioscience and Biotechnology Research, Rockville, MD
- WP 321 **Phosphoform-Specific Characterization of Protein Conformational Changes Induced by Multisite Phosphorylation;** Jingxi Pan¹; Albert Chou¹; Suping Zhang²; Christoph H. Borchers^{1,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²MRM Proteomics Inc, Victoria, BC, Canada; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- WP 322 **Top-Down Analysis of 'On-the-Fly' HDX of Native Protein Ions;** Ken Chanthamontri¹; Nawaporn Sanguantrakun^{2,3}; Michael L Gross³; ¹Washington University in St Louis, St Louis, MO; ²Saint Louis College of Pharmacy, St. Louis, MO; ³Washington University in St. Louis, Saint Louis, MO

- WP 323 **HDXMS Studies of Membrane Proteins (GPCR) Expressed in Virus like Particles (VLP);** Deepa Balasubramaniam¹; Carrie A Shipley¹; Beata A Zamlynny¹; Margarita Garcia-Calvo¹; Payal Sheth¹; Michael Kavana¹; David G McLaren¹; ¹Merck Research Labs, Kenilworth, NJ
- WP 324 **HX-MS Reveals a Loss of Helical Structure in an Intrinsically Disordered Protein under Highly Crowded Conditions;** Farai Rusinga; University of Kansas, Lawrence, KS
- WP 325 **Observation of H/D Exchange at Non-labile C-H Sites Capable by an Increase in Desolvation Temperature in ESI-source;** Alexander Zhrebek^{1,2}; Yuri Kostyukovich^{2,3,4}; Alexey S Kononikhin^{2,4}; Vitaliy Roznyatovsky¹; Igor A Popov^{4,5}; Yuri K. Grishin¹; Irina V Perminova¹; Eugene Nikolaev²; ¹Lomonosov Moscow State University, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Skolkovo Institute of Technology, Moscow, Russia; ⁴Moscow Institute of Physics and Technology, Moscow, Russia; ⁵Emanuel Institute of Biochemical Physics, Moscow, Russia
- WP 326 **Towards a High Throughput Binding-Site Specific Drug Screening by HDX MS;** ROMAN ZUBAREV¹; Juan Astorga-Wells^{2,3,4}; Thorleif Lavold³; ¹Karolinska Institutet, Stockholm, Sweden; ²Karolinska Institutet, Solna, Sweden; ³Biomotif AB, Stockholm, Sweden; ⁴HDXperts AB, Stockholm, Sweden
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- WP 329 **Local Dynamics in Lipid-Associated Apolipoprotein A-I and Effects of Disease-Causing Mutations Probed by Hydrogen-Deuterium Exchange MS;** Christopher Jay Wilson¹; Madhurima Das²; Xiaohu Mei²; John R Engen¹; Olga Gursky²; ¹Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; ²Department of Physiology and Biophysics, Boston University School of Medicine, Boston, MA
- WP 330 **Integrating XL-MS and HX-MS2 Data to Develop a Model of DNA Binding to DNAPKcs;** Morgan Hepburn¹; Daniel Saltzberg²; Yapping Yu¹; Susan Lees-Miller¹; Andrej Sali²; David Schriemer¹; ¹University of Calgary, Calgary, Canada; ²University of California, San Francisco, CA
- WP 331 **Identification of a Structural Conduit for Thermal Energy Transfer from Solvent to Enzyme Active Site using Hydrogen/Deuterium Exchange Mass Spectrometry;** Anthony T Iavarone¹; Adam R Offenbacher¹; Judith P Klinman¹; ¹UC Berkeley, Berkeley, CA
- WP 332 **Examining the Importance of Conformational Dynamics for the Function of Pyruvate Kinase: Insights from HDX-MS;** Courtney S Fast¹; Siavash Vahidi¹; Stanley D Dunn¹; Lars Konermann¹; ¹Western University, London, Canada
- WP 333 **Analysis of HIV Nef Dimerization and Binding Partner Interactions by Hydrogen Exchange Mass Spectrometry;** Jamie Moroco¹; John Jeff Alvarado²; Thomas E Smithgall²; John R Engen¹; ¹Northeastern University, Boston, MA; ²University of Pittsburgh School of Medicine, Pittsburgh, PA
- WP 334 **Pre-Amyloid Oligomer Dissociation Kinetics Studied by Hydrogen/Deuterium Exchange Mass Spectrometry;** Zhe Zhang¹; Richard W Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- WP 335 **Gas-Phase H/D Exchange Monitored by MS Reveals a Dense Network of Side-Chain Interactions Stabilizing Oligomers of Alzheimer's Disease A β Peptide;** Kaja Przygonska¹; Kinga Fituch¹; Ewa Sitkiewicz¹; Kasper D Rand²; Michal Dadlez¹; ¹Institute of Biochemistry and Biophysics, Polish Academy of Science, Warsaw, Poland; ²Department of Pharmacy, University of Copenhagen Copenhagen, Denmark
- WP 336 **Effect of Protein Structure on Antibody Deamidation Rates: A Combination of Peptide Mapping, 3D Modeling, and Hydrogen/Deuterium Exchange Mass Spectrometry;** Paul Mawson; Ridgefield, CT
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- WP 338 **Selenium Accumulation and Speciation in Supplemented Aquaponic Systems Using Reverse Phase HPLC and ICP-QQQ;** Skyler Smith¹; Julio A. Landero-Figueroa¹; Megan Schmale¹; ¹University of Cincinnati, Cincinnati, OH
- WP 339 **Environmental Source Determination Using Stable Lead Isotope Ratios in American Woodcock (Scolopax minor) Feathers and Bone;** Amanda D. French¹; Warren C Conway¹; Daniel S Sullins²; David Klein³; ¹Texas Tech University, Lubbock, Texas; ²Kansas State University, Manhattan, KS; ³Texas Tech University, Lubbock, TX
- WP 340 **Rapid Determination of Calcium in Water by Spray Microwave Plasma Torch Mass Spectrometry;** Meiling Yang¹; Xinchun Wang¹; Tao Zhong¹; Huanwen Chen²; ¹East China Institute of Technology, Nanchang, China; ²East China University of Technology, Nanchang, Mainland China
- WP 341 **Determination of Absolute Isotopic Composition of Mo by MC-ICP-MS using Synthetic Isotope Mixtures and Uncertainty Evaluation;** Panshu Song¹; Jun Wang¹; ¹National Institute of Metrology, Beijing, China
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- WP 343 **Differential Protein Profiling using Virtual 2D Gel-Mass Spectrometry;** Neil R Quebbemann¹; Joseph A Loo¹; Rachel R. Ogorzalek Loo¹; ¹University of California, Los Angeles, Los Angeles, CA
- WP 344 **Targeted DESI Mass Spectrometry Imaging in Ovarian Cancer;** Luisa Doria¹; James McKenzie¹; Anna Mroz¹; Abigail Speller¹; Francesca Rosini¹; David Phelps¹; Emrys A Jones²; Renata Soares¹; Kirill Veselkov¹; Sadaf Ghaem-Maghani¹; Zoltan Takats¹; ¹Imperial College, London, UK; ²Waters, Manchester, UK
- WP 345 **Tissue Imaging with Specificity for Unsaturated Lipid Isomers Using Mass Spectrometry with Photochemical Reactions;** Chengan Guo¹; Xiaoxiao Ma²; Yuan Su²; Ran Tian²; Ruyi Shi²; Fei Tang¹; Yu Xia²; Zheng Ouyang²; ¹Tsinghua University, Beijing, China; ²Purdue University, West Lafayette, IN

- WP 346 **Methodology for Drug Delivery Quantitation in Single Cells using TOF-SIMS**; Anthony Castellanos¹; Quentin Vanbellingen¹; Francisco Fernandez-Lima^{1,2}; ¹Florida International University, Miami, FL; ²Biomolecular Science Institute, Miami, FL
- WP 347 **Single Cell Analysis using nano-DESI Mass Spectrometry**; Hilde-Marlene Bergman¹; Ingela Lanekoff¹; ¹Uppsala University, Uppsala, Sweden
- WP 348 **Region- and Enzyme-Specific Bioconversion of Dynorphin Neuropeptide Detected by *in situ* Histochemistry and MALDI Imaging Mass Spectrometry**; Erik Bivehed¹; Stromvall Robert¹; Malin Andersson¹; ¹Uppsala University, Uppsala, Sweden
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- WP 350 **Tissue Classification using Mass Spectrometry and Membrane Microarrays**; Jone Garate¹; Roberto Fernandez²; Tarson Tolentino-Cortez²; Sergio Lage¹; Gabriel Barreda-Gómez²; Egoitz Astigarraga²; Jose A Fernandez¹; ¹University of Basque Country, UPV/EHU Leioa Basque Country, Spain; ²IMG Pharma Biotech, Zamudio, Spain
- WP 351 **Ambient Ionization Mass Spectrometry for Preoperative Diagnosis of Indeterminate Thyroid Nodules**; Jialing Zhang¹; Wendong Yu²; Clara L Feider³; Jerry Buentello²; Robert Tibshirani⁴; James W Suliburk²; Livia S Eberlin³; ¹UT Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX; ³University of Texas at Austin, Austin, TX; ⁴Stanford University, Stanford, CA
- WP 352 **Mass Spectrometry Imaging of the Human Pancreas Lipidome**; Grant Barry¹; Daniel Cavazos¹; Igor Vervovkin¹; Manami Hara²; Graeme Bell²; Luke Hanley¹; ¹University of Illinois at Chicago, Chicago, IL; ²University of Chicago, Chicago, IL
- WP 353 **Simultaneous Detection and Imaging of Drugs and Delivery Vehicles using LDI-MS**; Bo Zhao¹; Mine Canakci¹; Sankaran Thayumanavan¹; Richard W Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- WP 354 **Polarity Switching and Quantitative Mass Spectrometry Imaging of Healthy and Cancerous Hen Ovarian Tissue Sections using IR-MALDESI**; Milad Nazari¹; Mark T Bokhart¹; Kenneth P Garrard¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC
- WP 355 **Rapid Detection and Imaging of Fire-Retardant-Cyclodextrin-Inclusion Complexes on fibers and films by using IR-MALDESI Mass Spectrometry**; Yufei Chen¹; Nanshan Zhang¹; Milad Nazari¹; Mark Bokhart¹; Maans Ekeloef¹; David C Muddiman¹; Nelson R Vinuesa¹; ¹North Carolina State University, Raleigh, NC
- WP 356 **Metabolomic Imaging of Biofilm and Other Biological Materials for Studying Metabolomic Heterogeneity**; Tomasz Ruman¹; Joanna Nizioł¹; Vincent Bonifay¹; Jon Brauer¹; Christine Gaylarde¹; Iwona B Beech¹; Jan A Sunner¹; ¹University of Oklahoma, Norman, OK
- WP 357 **Matrix-free Analysis of Resveratrol in Intact Rat Retina Tissue Using REDichip**; Amanda Martinez¹; Andrea Kelley¹; Madeline Colley¹; Stephan Bach¹; ¹University of Texas at San Antonio, San Antonio, TX
- WP 358 **Lanthanide Labeled Antibody Detection by SIMS nano-TOF II of Human Intestinal Injury Markers**; Keely Pierzchalski; Maastricht, Limburg
- WP 359 **Mass Spectrometric and FT-IR Spectroscopic Imaging to Probe Organic Ligands and Their Binding Schemes on Nanocrystals**; Tae Lee¹; Jin Gyeong Son²; Jeong Hee Moon³; Sang Woo Han²; ¹KRISS, Daejeon; ²KAIST, Daejeon, Republic of Korea; ³KRIBB, Daejeon, Republic of Korea
- WP 360 **Analysis of Medical Devices in 2D and 3D by Secondary Ion Mass Spectrometry**; Adam Taylor¹; Felicia Green¹; Bonnie Tyler¹; Josephine Bunch¹; ¹National Physical Laboratory, Teddington, UK
- WP 361 **Multiplex Proteins and Lipids SIMS Imaging of Mouse Hippocampus Tissues**; Eunseok Seo¹; Sun young Lee¹; Young-ho Park¹; EunSook Choi¹; EunJoo Kim¹; Dong Kwon Lim²; Su-Il In¹; DaeWon Moon¹; ¹DGIST, Daegu, Korea; ²Korea University, Seoul, Korea
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- WP 363 **Precursor Ion Selector Scan for Discovery of Analyte Specific Fragments in MALDI-TOF/TOF-MS/MS**; Stanislav Rubakhin¹; Jonathan V Sweedler²; ¹Beckman Institute, UIUC, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- WP 364 **MS Imaging to Analyse the Transition from Early Goal-Directed Phase to Late Habituation Phase of Spatial Learning in Mice**; Geert Baggerman^{1,2}; Jeroen Aerts³; Laurens Minerva³; Dirk Valkenburg^{1,2,4}; Annelies Laeremans³; D'hooge Rudi³; Kurt Boonen³; Lutgarde Arckens³; ¹Flemish Institute for Technological Research (VITO), Mol, Belgium; ²University of Antwerp, Antwerp, Belgium; ³KU Leuven, Leuven, Belgium; ⁴Hasselt University, Diepenbeek, Belgium

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- WP 367 **Improved Qualitative and Quantitative Analysis of the Human Mitochondrial Proteome by Hybrid Acquisition**; Maurizio Ronci¹; Enrico Cilio¹; Steven Ciavarini²; Curt Devlin²; Brad Williams²; Scott Geromanos²; Chris Hughes³; Johannes Vissers⁴; Andrea Urbani¹; ¹University of Rome Tor Vergata, Rome, Italy; ²Waters, Milford, MA; ³Waters, Wilmslow, UK; ⁴Waters Corporation, Wilmslow, Greater Manchester
- WP 368 **Development of MSn Spectral Database and the Search Algorithm using Multiple MSn Spectra**; Yohei Yamada¹; Akemi Suzuki²; Umemura Yoshikatsu¹; Hiroyuki Yasuda¹; Yutaro Yamamura¹; Hideshi Fujiwaki¹; Kageyama Tetsuya¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Tohoku Pharmaceutical University, Miyagi, Japan
- WP 369 **Analysis of Polarity-Switched DESI Images of Colorectal Tissue Samples**; James Stuart McKenzie¹; Anna K Mróz¹; Renata Filipe-Soares¹; Zoltan Takats¹; ¹Imperial College, London, UK
- WP 370 **Mass Graph-Based Proteoform Identification by Top-Down Mass Spectrometry**; Qiang Kou¹; Si Wu²; Nikola Tolic³; Ljiljana Pasa-Tolic³; Xiaowen Liu^{4,5}; ¹Indiana University-Purdue University, Indianapolis, IN; ²University of Oklahoma, Dept. of Chem & Biochem Norman, OK; ³Pacific Northwest National Laboratory, Richland, WA; ⁴Indiana University-Purdue University Indianapolis, Indianapolis, IN; ⁵Indiana University School of Medicine, Indianapolis, IN



- WP 371 **A Very Fast Bayesian Engine for Truly unified MS1- and MS2-based Protein Inference**; Julianus Pfeuffer¹; Xiao Liang²; Knut Reinert²; Oliver Kohlbacher¹; Oliver Serang³; ¹Eberhard Karls Universität Tübingen, Tübingen, BW, Deutschland; ²Freie Universität Berlin, Berlin, Germany; ³Freie Universität Berlin, Berlin
- WP 372 **An Adjusted-Median Approach to Missing Values in Label Free Quantitation**; Seth Just¹; Luisa Zini¹; Nick Vincent-Maloney¹; Brian C Searle^{1,2}; ¹Proteome Software, Portland, OR; ²University of Washington, Seattle, WA
- WP 373 **Machine Learning Algorithms for Advanced Identification of Tumor Tissue and Tumor Borders**; Evgeny Zhvansky^{1,2}; Igor A Popov^{1,2}; Anatoly Sorokin¹; Nikita Levin¹; Vsevolod Shurkhay³; Denis Bormotov¹; Maria Indeykina^{2,4}; Alexey S Kononikhin^{2,4}; Yuri Kostyukovich^{2,4}; Evgeny Kukaev^{1,2}; Alexander Potapov³; Eugene Nikolaev²; ¹Moscow Institute of Physics and Technology, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics, Moscow, Russia; ³Burdenko Neurosurgical Institute, Moscow, Russian Federation; ⁴Emanuel Institute of Biochemical Physics, Moscow, Russia
- WP 374 **Making the Most of Multi-Modality Imaging: Exploring Fusion of Mass Spectrometry Imaging with Stimulated Raman Spectroscopy**; Alan Race¹; Alasdair Rae²; Jean-Luc Vorng²; Rory Steven²; Josephine Bunch²; Ian Gilmore²; ¹National Physical Laboratory, Teddington, Middlesex; ²National Physical Laboratory, Teddington, UK
- WP 375 **Automated Tumor Typing of Tissue Sections Based on Characteristic Spectral Patterns Extracted from MALDI Mass Spectrometry Imaging Data**; Tobias Boskamp^{1,2}; Delf Lachmund¹; Nicolas Jathe¹; Christian Etman¹; Janina Oetjen¹; Rita Casadonte³; Jan Hendrik Kobarg²; Dennis Trede²; Jörg Kriegsmann^{3,4}; Peter Maass^{1,2}; ¹University of Bremen, Bremen, Germany; ²SciLS GmbH, Bremen, Germany; ³Proteopath GmbH, Trier, Germany; ⁴Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany
- WP 376 **Virtual Lock Masses: An Algorithmic Method to Enable Mass Spectra Comparison in Untargeted Studies**; Francis Brochu¹; Pier-Luc Plante^{1,2}; Alexandre Drouin¹; Louis-Émile Robitaille¹; François Lavolette¹; Mario Marchand¹; Jacques Corbeil^{1,2}; ¹Université Laval, Québec, Canada; ²Centre de Recherche du CHU de Québec, Québec, Canada
- WP 377 **Isotopic Tree: Fast Calculation of Fine and Coarse Isotopic Envelopes up to a Predefined Margin of Error**; Dmitry Avtonomov¹; Alexey I Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- WP 378 **DISCO - Data Independent Signal Correlator**; David Shteynberg¹; Samuel L Bader¹; Andrew Keller¹; Michael Hoopmann¹; Luis Mendoza¹; Eric Deutsch¹; Robert L Moritz¹; ¹Institute for Systems Biology, Seattle, WA
- WP 379 **A Parameterized Averaging Model Improves Feature Detection of Oligonucleotides and Increases Wider Applicability of Feature Finding Algorithm**; Samuel Wein¹; Benjamin A Garcia²; ¹University of Pennsylvania, Philadelphia, Pa; ²University of Pennsylvania, Philadelphia, PA
- WP 380 **MassTodon - Electron Transfer driven Fragmentation Analyzer and Automatic Spectrum Calibrator**; Mateusz Krzysztof Łacki^{1,2}; Frederik Lermyte^{3,4}; Michał Startek²; Dirk Valkenborg^{4,5,6}; Frank Sobott^{3,4}; Anna Gambin²; ¹University of Warsaw, Warszawa, Mazowieckie; ²Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ³Biomolecular & Analytical Mass Spectrometry group, University of Antwerp, Antwerpen, Belgium; ⁴UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; ⁵Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; ⁶VITO, Mol, Belgium
- WP 381 **IsoSpec - a Hyperfast Generator of Fine Isotopic Structure Peaks with Preset Total Probability**; Mateusz Krzysztof Łacki¹; Michał Startek¹; Dirk Valkenborg^{2,3,4}; Anna Gambin¹; ¹Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ²UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; ³Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; ⁴VITO, Mol, Belgium
- WP 382 **Robust Algorithms for Denoising, Eliminating Dispersion Similar to Phasing in 1D_FT-MS Spectra and Reconstructing Non Uniformly Sampled 2D_FT-ICR Data**; Lionel Chiron¹; Fabrice Bray²; Christian Rolando³; Marc-André Delsuc⁴; ¹CASC4DE, Strasbourg, France; ²Université de Lille, Villeneuve d'Ascq, France; ³Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq; ⁴Université de Strasbourg, Strasbourg, France
- WP 383 **Finding the Peaks: Performance Enhancement of Portable MS using a Bayesian Approach**; Simon Maher¹; Simon Maskell¹; Sarfaraz Syed²; Fred Jjunju¹; Stephen Taylor¹; ¹Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK; ²Maastricht University, Maastricht, NL
- WP 384 **Integrated GlycoProteome Analyzer (I-GPA) for Automatic Identification and Quantitation of Site-Specific N-Glycosylation**; Gun Wook Park^{1,2}; Jin Young Kim²; Heeyoun Hwang²; Ju Yeon Lee²; Young Hee Ahn³; Hyun Kyoung Lee²; Eun Sun Ji²; Hoi Keun Jeong²; Ki Na Yun²; Yong-Sam Kim⁴; Jeong-Heon Ko⁴; Hyun Joo An⁵; Jae Han Kim⁵; Young-Ki Paik⁶; Jong Shin Yoo²; ¹Chungnam National University, Cheongju, Chungbuk; ²Korea Basic Science Institute, Cheongju-Si, Republic of Korea; ³Cheongju University, Cheongju-Si, Republic of Korea; ⁴Korea Research Institute of Bioscience and Biotechnology, Daejeon, Republic of Korea; ⁵Chungnam National University, Daejeon, Republic of Korea; ⁶Yonsei University, Seoul, South Korea
- WP 385 **Identification of N-glycopeptides using Open Spectral Library Search**; Zhiwu An¹; Qingbo Shu¹; Hao Lv¹; Jianjun Yu¹; Fuquan Yang¹; Yan Fu¹; ¹Chinese Academy of Sciences, Beijing, Beijing
- WP 386 **Extending MS Interpreter: A Freely-Available Tool for Structure/Spectrum Self-Consistency of High Resolution Tandem Mass Spectra**; Alexey V. Mayorov^{1,2}; Yuri Mirokhin³; Dmitrii Tchekhovskoi³; Stephen Stein³; ¹NIST, Gaithersburg; ²N.M. Emanuel Institute of Biochemical Physics RAS (IBCP RAS), Moscow, Russian Federation; ³NIST, Gaithersburg MD
- WP 387 **Machine Learning-Driven Validation Platform for Mass Spectrometry Imaging using Tandem Mass Spectra and Chemical Structure Databases**; Ivan Laponogov¹; Emilie J L Cauet²; James McKenzie²; Robert C Glen²; Zoltan Takats²; Kirill Veselkov²; ¹Imperial College London, London, London; ²Imperial College, London, UK
- WP 388 **Improving LC-MS Coverage through New Charge State and Monoisotopic m/z Assignment Algorithms**; Graeme McAlister¹; Derek Bailey¹; Romain Huguet¹; Michael Senko¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 389 **SAINTq: Robust Scoring of Protein-Protein Interactions in Quantitative AP-SWATH Experiments**; Guoci Teo¹; Hiromi WL Koh¹; Damian Fermin²; Jean-Philippe Lambert³; James Knight³; Anne-Claude Gingras³; Hyungwon Choi⁴; ¹National University of Singapore, Singapore, Singapore; ²Yale University, New Haven, CT; ³Lunenfeld Tanenbaum Research Institute, Toronto, Canada; ⁴National University of Singapore, Singapore



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- WP 390 **Galaxy-P: Recent Developments and Emerging Applications**; Pratik Jagtap^{1,2}; James Johnson³; Thomas McGowan³; Innocent Onsong³; Benjamin Lynch³; Candace Guerrero¹; Kevin Murray¹; Lloyd M Smith⁴; Michael R Shortreed⁴; Anthony J Cesnik⁴; Lennart Martens^{5,6}; Adrian Hegeman¹; Timothy Griffin^{1,2}; ¹University of Minnesota, Minneapolis, MN; ²Center for Mass Spectrometry and Proteomics, UMN St. Paul, MN; ³University of Minnesota Supercomputing Institute, Minneapolis, MN; ⁴University of Wisconsin Madison, Madison, Wisconsin; ⁵Ghent University, Ghent, Belgium; ⁶VIB, Ghent, Belgium
- WP 391 **Optide-Hunter: Informatics Solutions for Optimized Peptide Drug Development through the Integration of Heterogeneous Data and Adaptation of Various LC-MS Technologies**; Mi-Youn Brusniak¹; Emily Girard¹; Bernard Lee²; Chris Mehlin¹; Yuko Ogata¹; Philip Gafken¹; Hector Ramos¹; Jim Olson¹; ¹Fred Hutchinson Cancer Research Center, Seattle, WA; ²LabKey Software, Seattle, WA
- WP 392 **APOSTL: An interactive Galaxy Pipeline For Reproducible Analysis of Affinity Proteomics Data**; Brent Kuenzi¹; Adam Borne¹; Jiannong Li¹; Uwe Rix¹; Paul Stewart¹; Eric Haura¹; ¹H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL
- WP 393 **Enabling Collaborative Discovery in Big Data Visual Analytics**; Joon-Yong Lee¹; Ryan Wilson¹; Grant M Fujimoto¹; Gary R Kiebel¹; Richard D Smith¹; Nick Cramer¹; Samuel H Payne¹; ¹Pacific Northwest National Lab, Richland, WA
- WP 394 **Scientific Workflows for Data Analysis and Visualization in Quantitative Proteomics**; Arzu Tugce Guler¹; Dmitrii Travin²; Yassene Mohammed¹; Magnus Palmblad¹; ¹Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands; ²Faculty of Bioengineering and Bioinformatics, Lomonosov Moscow State University, Moscow, Russia
- WP 395 **Integration of Peptide-Centric Searching of Data Independent Acquisition Data without an MS/MS Spectrum Library with Data in the Chorus Project**; Michael J. MacCoss¹; Brian C Searle¹; Sonia Ying Ting¹; Jarrett Egerton¹; Christine C Wu²; Andrii Laboda³; Oleksii Tymchenko³; Andrey Bondarenko³; ¹Univ of Washington, Seattle, WA; ²Stratus Biosciences, Seattle, WA; ³Infoclinika, LLC, Seattle, WA
- WP 396 **High Performance Computing at the National Resource for Translational and Developmental Proteomics**; Ryan T Fellers¹; Richard D LeDuc¹; Bryan P Early¹; Joseph B Greer¹; Alexandra J Van Nispen¹; Paul M Thomas¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL
- WP 397 **The MassIVE Repository for Interactive Annotation of Proteomics Big Data**; Jeremy Carver¹; Mingxun Wang¹; Nuno Bandeira¹; ¹UCSD, La Jolla, CA
- WP 398 **The Potential of Functional Annotation of Mass Spectrometry Tools**; Magnus Palmblad¹; Arzu Tugce Guler¹; Kristian Davidsen²; Jon Ison²; Veit Schwämmle³; ¹Leiden University Medical Center, Leiden, the Netherlands; ²Technical University of Denmark, Copenhagen, Denmark; ³University of Southern Denmark, Odense, Denmark
- WP 399 **Recent Developments in ProteomicsDB: From FDR Estimates to Proteomic Assays and More**; Mathias Wilhelm¹; Daniel Paul Zolg¹; Hans-Christian Ehrlich²; Stephan Aiche²; Mohammed AbuJarour²; David Weese²; Judith Schlegl³; Tobias Schmidt¹; Wilhelm Becker²; Lars Rückert²; Jan Huenges²; Susan Klaeger^{1,4,5}; Stephanie Heinzlmeir^{1,4,5}; Hannes Hahne^{1,6}; Bernhard Kuster^{1,4,5}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²Innovation Center Potsdam, SAP SE, Potsdam, Germany; ³SAP SE, Walldorf, Germany;

⁴German Cancer Consortium (DKTK), Muenchen, Germany;
⁵German Cancer Research Center, Heidelberg, Germany;
⁶OmicScouts GmbH, Freising, Germany

- WP 400 **Dredging the Mass Spectrometry Data Lake for Hidden Information with Teradata Database and Business Intelligence Software**; Alan Dickson¹; Tony Ly¹; Vackar Afzal¹; Dalila Bensaddek¹; Jens Hukelmann¹; Angus Lamond¹; ¹Centre for Gene Regulation and Expression, Dundee, UK
- WP 401 **Comparison of Data Processing Strategies for Optimal Detection of Protein-Protein Interactions**; Gerhard Duernberger^{1,2}; Florian Stanek³; Johannes Doblmann³; Zuzana Demianova³; Karl Mechtler³; ¹GMI - Gregor Mendel Institute of Molecular Plant Biology, Vienna, Austria; ²IMP - Research Institute of Molecular Pathology, Vienna, Vienna; ³IMP - Research Institute of Molecular Pathology, Vienna, Austria
- WP 402 **Proteomics in Perl: A Streamlined Approach**; Jeremy D Volkening¹; Michael R Sussman¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 403 **RAId GUI: A Graphical User Interface for RAId Tandem Mass-Spectrometry Database Search Tool**; Danny Lee¹; Aleksey Ogurtsov¹; Gelio Alves¹; Yi-Kuo Yu¹; ¹National Center for Biotechnology Information, NLM, NIH, Bethesda, MD
- WP 404 **Xcalibur Workbench: A Lua Based Data Browser**; Michael W. Senko¹; Graeme C McAlister¹; Derek Bailey¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 405 **CHORUS is Innovative and User Friendly Platform for Third Party Mass Spectrometry Software Integration**; Andrey Bondarenko¹; Andrii Laboda^{1,2}; Oleksii Tymchenko^{1,2}; Vladimir Moiseiev^{1,2}; Nathan Yates³; Mai Sun³; Michael J MacCoss⁴; Brendan Maclean⁴; Christine Wu⁴; Brian C Searle⁴; Sonia Ying Ting⁴; Jimmy K Eng⁴; Nick Shulman⁴; Juergen H Cox⁵; Chris Becker⁶; ¹InfoClinika, Bellevue, WA; ²TeamDev, Kharkiv, Ukraine; ³University of Pittsburgh, Pittsburgh, PA; ⁴University of Washington, Seattle, WA; ⁵Max Planck Institute for Biochemistry, Martinsried, Germany; ⁶Protein Metrics Inc., San Carlos, CA

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS

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- WP 406 **Fingerprinting of Falsified Artemisinin Combination Therapies (ACTs) via DART Ionization Coupled to a Compact Single Quadrupole Mass Spectrometer**; Matthew Bernier¹; Frederick Li²; Joseph LaPointe²; Brian D Musselman²; Paul Newton^{3,4}; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²IonSense, Inc. Saugus, MA; ³Lao-Oxford-Mahosot Hospital Wellcome Trust Research Unit (LOMWRU), Vientiane, Laos; ⁴Centre for Tropical Medicine and Global Health, University of Oxford, Oxford, UK
- WP 407 **Explosive Detection Using a Portable Benchtop Cylindrical Ion Trap-Mass Spectrometer**; Stephen Davila¹; Corey Stedwell¹; Daniel DeBord¹; ¹1st Detect Corporation, Webster, TX
- WP 408 **Establishing a Baseline for a Portable Stable Carbon Isotope Detection System**; Brian Thomas¹; Steve Taylor¹; Tim Clarey²; Dave McIntosh¹; ¹University of Liverpool, Liverpool, UK; ²The King's University, Southlake, TX
- WP 409 **Micro Mass Spectrometer Approach for Cometary Exploration**; Ashish Chaudhary¹; Friso van Amerom¹; Tim Short¹; Emily Barrentine²; Yun Zheng²; Daniel Glavin²; William Brinckerhoff²; Paul Mahaffy²; ¹SRI International, St. Petersburg, FL; ²NASA GSFC, Greenbelt, MD
- WP 410 **Development of Compact Laser Desorption/Ionization Time-of-Flight Mass Spectrometer for Planetary Missions**; Xiang Li¹; Stephanie Getty²; Andrej Grubisic³; Kyle Uckert⁴; William Brinckerhoff²; Timothy J Cornish⁵;



- Scott Ecelberger⁵; ¹University of Maryland, Baltimore County, Greenbelt, MD; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³University of Maryland, College Park, College Park, MD; ⁴New Mexico State University, Las Cruces, NM; ⁵C&E Research, Inc, Columbia, MD
- WP 411 **Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer: Performance Testing in GC-MS and LD-MS Modes of Operation;** Veronica Pinnick¹; Ryan Danell²; Friso van Amerom³; Samuel Larson³; Arnaud Buch⁴; Cyril Szopa⁵; Xiang Li¹; Andrej Grubisic⁶; Ricardo Arevalo³; Stephanie Getty³; William Brinckerhoff³; Paul Mahaffy³; Francois Raulin⁷; Fred Goesmann⁸; ¹University of Maryland, Baltimore County Greenbelt, MD; ²Danell Consulting, Inc. Winterville, NC; ³NASA GSFC, Greenbelt, MD; ⁴Ecole Centrale, Paris, France; ⁵Laboratoire Atmosphères, Paris, France; ⁶University of Maryland, College Park, MD; ⁷Laboratoire Interuniversitaire des Systèmes Atmosphériques, Paris, France; ⁸Max Planck Institut für Sonnensystemforschung, Göttingen, Germany
- WP 412 **Characterization of the Mars Organic Molecule Analyzer Mass Spectrometer Intrinsic Dynamic Range;** Friso H.W. Van Amerom¹; Xiang Li²; Ryan Danell³; Veronica T Pinnick²; Stephanie Getty⁴; Ricardo Arevalo⁴; Andrej Grubisic⁵; Lars Hovmand⁶; William Brinckerhoff⁴; Paul Mahaffy⁴; Fred Goesmann⁷; ¹Mini-Mass Consulting, Inc, Hyattsville, MD; ²University of Maryland, Baltimore County Greenbelt, MD; ³Danell Consulting, Winterville, NC; ⁴NASA GSFC, Greenbelt, MD; ⁵University of Maryland, College Park, MD; ⁶Linear Labs, Washington DC; ⁷Max Planck Institut für Sonnensystemforschung, Goettingen, Germany
- WP 413 **The Europa Mass Spectrometer for Planetary Exploration (MASPEX). A High-Resolution Multi-Pass Time-of-Flight Mass Spectrometer;** Gregory P. Miller¹; Jack Hunter Waite, Jr.²; Tim Brockwell²; John Roberts²; Keith S Pickens²; Ryan C. Blase²; Paul Wilson V²; ¹Southwest Research Institute, San Antonio, TX; ²Southwest Research Institute, San Antonio, TX
- WP 414 **Silence is Golden: Detector Radiation Shielding at Europa for MAss Spectrometer for Planetary EXploration (MASPEX);** Ryan C. Blase¹; Roland R. Benke²; Keith S. Pickens¹; Gregory P. Miller¹; Tim Brockwell¹; John Roberts¹; Paul Wilson IV¹; J.H. Waite, Jr.¹; ¹Southwest Research Institute, San Antonio, TX; ²Atom Consulting LLC / Consultant to SwRI, Austin, TX
- WP 415 **Development of an Integrated LC-MS Prototype for an *in situ* Mission to an Icy Body in the Solar System;** Adrian Southard¹; Stephanie Getty²; Jerome P Ferrance³; Brian N Stamos⁴; Jamie E Elsil²; Manuel A Balvin²; Daniel P Glavin²; Daniel S Stewart²; Brandon J Colon-Curiel⁵; ¹Universities Space Research Association, Columbia, MD; ²NASA GSFC, Greenbelt, MD; ³J2f engineering, Charlottesville, VA; ⁴University of Texas at Arlington, Arlington, TX; ⁵University of Puerto Rico Mayaguez, Mayaguez, PR
- WP 416 **Towards Remote Chemical Sensing Using an Aerodynamic Assisted Portable Mass Spectrometer;** Yanbing Zhai¹; Ting Jiang¹; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, China
- WP 417 **Portable Multiple Ionization Sources Biological Mass Spectrometer;** Jung-Lee Lin¹; Ming-Lee Chu¹; Chung-Hsuan Chen¹; ¹Academia Sinica, Taipei, Taiwan
- WP 418 **Low Temperature Co-fired Ceramic (LTCC)-Packaged MEMS Micro-ion Source for Miniature Mass Spectrometry Applications;** Charles B Parker¹; Erich J Radauscher¹; Kristin H Gilchrist²; Shane DiDona¹; Zachary E Russell¹; Stephen D Hall²; James B Carlson²; Sonia Grego²; Steven J Edwards³; Roger P Sperline³; M. Bonner Denton³; Brian R Stoner^{1,2}; Jeffrey T Glass¹; Jason J Amsden¹; ¹Department of Electrical and Computer Engineering, Duke University, Durham, NC; ²Engineering and Applied Physics Division, RTI International, Research Triangle Park, NC; ³Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ
- WP 419 **Handheld and Portable DAPCI Source for Point and Shoot Applications: Towards Onsite *in-situ* Explosives Analysis;** Fred Paul Mark Jjunju¹; Simon Maher²; Stephen Taylor^{2,3}; Graham R Cooks⁴; ¹Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK; ²University of Liverpool, Liverpool, UK; ³Q-Technologies Ltd, Liverpool, UK; ⁴Department of Chemistry Purdue University, West Lafayette, IN
- WP 420 **Development of HPLC Methods for Use with Mobile Ambient Ionization Mass Spectrometry;** Leonard Rorrer.III¹; Mitch Wells¹; ¹FLIR Systems, Inc., West Lafayette, IN
- WP 421 **Improving the Selectivity of a High Pressure Mass Spectrometry;** Andrew Hampton; UNC - Chapel Hill, Chapel Hill, NC
- WP 422 **Falling Through the Cracks: High Resolution Quadrupole Mass Spectrometry;** Dave McIntosh¹; Mariya Antony-Joseph¹; Simon Maher¹; John Ray Gibson¹; Stephen Taylor¹; ¹University of Liverpool, Liverpool, UK
- WP 423 **Utilizing Silicon on Insulator Materials to Fabricate Miniature Ion Traps for High Pressure Mass Spectrometry;** Zachary Dyer¹; Craig Cavanaugh²; Kenion Blakeman²; Tina Stacy¹; Michael J Ramsey¹; ¹UNC Ramsey Group, Chapel Hill, NC; ²University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 424 **Miniaturized Toroidal Ion Trap using Cylindrical Electrodes;** Daniel Austin¹; Jessica Higgs¹; Kit White¹; Yuan Tian¹; ¹Brigham Young University, Provo, UT
- WP 425 **Overcoming the Tradeoff between Resolution and Sensitivity in Miniature Mass Spectrometry using Spatially Coded Apertures;** Zachary E Russell^{1,2}; Evan X Chen¹; Shane T DiDona¹; Jason J Amsden¹; Charles B Parker¹; Scott D Wolter³; Ryan M Danell⁴; Brian R Stoner⁵; Gottfried Kibelka⁶; Michael E Gehm¹; David W Brady¹; Jeffrey T Glass¹; ¹Duke University, Durham, NC; ²Stanford University, Stanford, CA; ³Elon University, Elon, NC; ⁴Danell Consulting, Inc. Winterville, NC; ⁵RTI International, Raleigh, NC; ⁶Xylem/OI Analytical, College Station, TX

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- WP 426 **Coupling Thin-Layer Chromatography with Matrix Assisted Inlet Ionization for Small Molecule Analysis;** Khoa Hoang¹; Charles N McEwen^{2,3}; ¹MSTM, Philadelphia, PA; ²University of the Sciences in Philadelphia, Philadelphia, PA; ³MSTM, LLC. Hockessin, DE
- WP 427 **Interfacing UPLC to Mass Spectrometry via a Liquid-junction, Secondary Ultrasonic API Source;** Steve Bajic¹; David S Douce¹; Gordon A Jones¹; ¹Waters Corporation, Manchester, England
- WP 428 **Development and Optimization of an Inlet System for Desorption Atmospheric Pressure Photoionization – Mass Spectrometry (DAPPI-MS);** Kai Kroll¹; Christine Polaczek¹; Tiina Kaupilla²; Anu Vaikkinen²; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany; ²University of Helsinki, Helsinki, Finland
- WP 429 **Glove Box MS Interface for the Measurement of Reaction Kinetics of Air-sensitive Compounds;** Alan T. Taylor¹; Ruth Dooley²; Mark Baumer³; Clive Aldcroft³; Mark Allen³; C. Logan Mackay²; Guy Lloyd-Jones²; ¹University of Edinburgh, Edinburgh, Lothian; ²School of Chemistry, The University of Edinburgh Edinburgh, UK; ³Advion UK Ltd, Essex, UK



- WP 430 **Volatile Terpene Analysis in Cannabis, Spices and Fresh Produce by Tandem Mass Spectrometry Fitted with a Modified Plasma Source;** Frank Kero¹; Craig Young¹; Heather Gamble²; Joshua Ye²; Lisa Cousins²; Chuck Joliffe²; Chai Yuan-Cheng³; Lin Jing-Chao³; ¹PerkinElmer, Downers Grove, IL; ²Ionics, Bolton, Canada; ³PerkinElmer, Shanghai, China
- WP 431 **A New Interface Design for Coupling a Liquid Stream to an Electron Ionization Source;** Alexander Lekkas¹; Dimitris Papanastasiou¹; Emmanuel Raptakis¹; Francesca Rigano²; Danilo Sciarra³; Luigi Mondello^{2,3}; ¹Fasmatech, Athens, Greece; ²Chromaleont s.r.l., Messina, Italy; ³Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Messina, Italy
- WP 432 **LC-MS with Cold EI – The New System and Recent Applications;** Svetlana Tsizin¹; Aviv Amirav²; Alexander B Fialkov¹; Tal Alon¹; ¹Tel Aviv University, Tel Aviv, Israel; ²Tel Aviv University, Tel-Aviv
- WP 433 **Study of Vaporization Surfaces in Liquid Chromatography – Electron Ionization Mass-Spectrometry;** Federica Bianchi¹; Laura Magrini²; Nicolò Riboni¹; Maria Careri¹; Achille Cappiello²; ¹University of Parma, Parma, Italy; ²University of Urbino, Urbino, Italy
- WP 434 **DEI vs. LEI: A Novel, Advanced System for Interfacing Liquid Chromatography and Electron Ionization Mass Spectrometry;** Achille Cappiello¹; Maurizio Piergiovanni¹; Giorgio Famiglini¹; Veronica Termopoli¹; Pierangela Palma¹; ¹University of Urbino, Urbino, Italy
- WP 435 **Evaluation of an Induction-Based Fluidics System for Delivery of Low Volume (nL) Samples;** Kelly Hanssen Smith¹; Susan M Schulz¹; Bryce F Doxzon¹; Ernest H Braue¹; Irwin Koplavitz¹; Kathleen Housman¹; Lee I Roberts¹; Jonathan Oylor¹; ¹USAMRICD, Aberdeen Proving Ground, MD
- WP 436 **AP-to-vacuum Inlet with New Features - Optimization of Desolvation Conditions in Liquid AP-MALDI MS;** Jeff Brown^{1,2}; Pavel Ryumin¹; Michael Morris²; Rainer Cramer¹; ¹University of Reading, Reading, UK; ²Waters, Wilmslow, UK
- WP 437 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Time of Flight Mass Spectrometry (GC-TOF-MS) for Identification and Quantification of Halogenated Compounds;** Kunyu Zheng¹; Hamid Badiei²; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC; ²PerkinElmer, Woodbridge, ON
- WP 438 **A Novel Method for Online Analysis of Electronic Cigarette Aerosol;** Christian Lindinger¹; Alfons Jordan¹; Philipp Sulzer¹; Kostiantyn Breiev¹; Kerstin M.M. Burseg²; Grant O'Connell²; Eugen Hartungen¹; Stefan S. Biel²; Xavier Cahours³; Stephane Colard³; Tilmann D. Märk^{1,4}; ¹IONICON Analytik GmbH., Innsbruck, AUSTRIA; ²Fontem Ventures B.V., Amsterdam, The Netherlands; ³SEITA - Imperial Tobacco Group, Fleury-les-Aubrais, France; ⁴Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens Universität Innsbruck, Innsbruck, Austria
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- WP 439 **Collision Cross Section (CCS) Measurements for Small Molecular Mixture by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Hu Miao¹; Zhang Linzhou¹; Xu Chunming¹; Quan Shi²; ¹China University of Petroleum, Beijing, China; ²State Key Laboratory of Heavy Oil Processing, Changping, Beijing
- WP 440 **Assessment of using Projection Superposition Approximation (PSA) with Molecular Modeling to Compute Collision Cross Sections For Ion Mobility Spectrometry;** Glenn Spangler; Technispan LLC, Lutherville, MD
- WP 441 **Predicting Theoretical Collision-cross Sections for Peptides and Peptide Fragments;** Bela Paizs¹; Oscar Hernandez²; Daniel Chaplin¹; Ash Buck¹; Keith Richardson²; Jeff Brown²; Kevin Giles²; Zoltan Takats³; ¹Bangor University, Bangor, UK; ²Waters, Wilmslow, UK; ³Imperial College, London, UK
- WP 442 **Evaluation of Collision Cross Section Measurements Obtained by Uniform Field Drift Tube IM-MS: Insight into Instrument Settings and Theoretical Calculations;** Sarah Stow¹; Jody C May¹; James N Dodds¹; Andrzej Balinski¹; Emma E Rennie²; Ruwan T Kurulugama²; John Fjeldsted²; John A McLean¹; ¹Vanderbilt University, Nashville, TN; ²Agilent Technologies, Santa Clara, CA
- WP 443 **Hide-and-Seek: The effect of Localisation of Partial Charges on Ions on Their Calculated CCS Values;** Lukasz Grzegorz Migas¹; Eleanor Sinclair¹; Christopher Gray¹; Sabine Flitsch¹; Perdita Barran¹; ¹University of Manchester, Manchester, UK
- WP 444 **On the Structural Denaturation of Biological Analytes in Trapped Ion Mobility Spectrometry - Mass Spectrometry;** Fanny Caroline Liu¹; Samuel R. Kirk¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- WP 445 **Collision Cross Section Accuracy of Common MS Calibrants Across a Large Number of Measurements in Positive and Negative Ion Modes;** Jody C. May¹; Ruwan T Kurulugama²; George C Stafford²; John C Fjeldsted²; John A McLean¹; ¹Vanderbilt University, Nashville, TN; ²Agilent Technologies, Santa Clara, CA
- WP 446 **Elucidating the Structural Heterogeneity of Biomolecules in the Gas Phase using Traveling Wave Ion Mobility Arrival Time Distributions;** Sugyan Dixit¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- WP 447 **Towards using Trapped IMS in Structural Biology Applications;** Christian Bleiholder¹; Fanny C Liu²; Samuel R Kirk²; Meggie Young²; Mengqi Chai²; ¹Florida State University, Tallahassee, FL; ²Florida State University, Tallahassee, FL
- WP 448 **Characterizing Instrumental Parameters in Trapped Ion Mobility Spectrometry (TIMS) for Transmission and Preservation of Native Analyte Structures and Their Complexes;** Samuel Kirk¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- WP 449 **Fundamentals of Trapped Ion Mobility Spectrometry: Fluid Dynamics;** Melvin A. Park¹; Karsten Michelmann²; Mark E Ridgeway¹; Joshua Silveira¹; ¹Bruker Daltonics, Inc., Billerica, MA; ²Bruker Daltonik GmbH, Bremen, Germany
- WP 450 **Decomposition Pathways during Explosive Analysis Using TIMS-MS and Molecular Dynamics;** Alan McKenzie¹; Mark E Ridgeway²; Melvin Park²; Francisco Alberto Fernandez Lima³; ¹Florida Int'l University, Miami, FL; ²Bruker Daltonic, Billerica, MA; ³Florida International University, Miami, FL
- WP 451 **Improving Ion Mobility – Mass Scan for the High Performance Ion Mobility Spectrometry – Mass Spectrometry;** Jianglin Wu¹; Adam M Graichen¹; Mark Osgood¹; Ching Wu¹; ¹Excellims Corporation, Acton, MA
- WP 452 **Structures for Lossless Ion Manipulations (SLIM) using Multilevel Traveling Wave Ion Escalators for Obtaining Ultrahigh Resolution Ion Mobility Separations;** Ahmed M Hamid¹; Yehia M Ibrahim¹; Sandilya V. B Garimella¹; Ian K Webb¹; Liulin Deng¹; Gordon A Anderson¹; Spencer A Prost¹; Jeremy A Sandoval¹; Randolph V Norheim¹; Erin S Baker¹; Richard D Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA
- WP 453 **Development and Evaluation of Long Serpentine Path Traveling Wave SLIM Modules for High Resolution Ion Mobility Separations;** Liulin Deng¹; Yehia M Ibrahim²; Ahmed M Hamid²; Sandilya Garimella²; Ian Webb²; Xing Zhang²; Tsung-Chi Chen²; Xueyun Zheng²; Erin Baker²;



- Richard D Smith²; ¹Pacific NW National Laboratory, Richland, WA; ²Pacific Northwest National Lab, Richland, WA
- WP 454 **Comparing Ion Multiplexing Techniques: Tangible Enhancement for Ion Mobility-Mass Spectrometry**; Brian H. Clowers¹; Austen L. Davis¹; Kelsey A Morrison¹; ¹Washington State University, Pullman, WA
- WP 455 **A Comparative Study of nanoESI and ESI on an Atmospheric Pressure High Performance Ion Mobility Spectrometer**; Mark Osgood¹; Adam M Graichen¹; Ching Wu¹; ¹Excellims Corporation, Acton, MA
- WP 456 **Modeling Space Charge Effects on the Performance of Transversal Modulation Ion Mobility Spectrometry: A Numerical Approach**; Cesar Barrios¹; Guillermo Vidal-de-Miguel²; ¹SEADM, Boecillo, Spain; ²Fossil Ion Technology S.L., Madrid, Spain
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- WP 460 **Comprehensive Electric Field Analysis of Resistive Glass Drift Tubes, Reflectrons, and Other Electro-Optical elements**; Robert Jackson¹; Matthew Breuer²; Paula Holmes²; Jeffrey DeFazio³; ¹Instrumental Design Physics, LLC, Littleton, MA; ²Photonis USA, Sturbridge, MA; ³PHOTONIS USA, Lancaster, PA
- WP 461 **Ion Mobility Coupled to Extended Mass Range Orbitrap for Structural Analysis of Large Proteins and Protein Complexes**; Michael Poltash¹; Kyle Fort²; David H Russell³; ¹Texas A&M University, College Station, Texas; ²Utrecht University, Utrecht, The Netherlands; ³Texas A&M University, College Station, TX
- WP 462 **Multistage Transversal Modulation IMS Coupled with IonMax Electrospray and Ion Trap MS to Provide a Modular ESI-IMS-MS Solution**; Guillermo Vidal-de-Miguel¹; Miriam Macia¹; Gonzalo Arranz²; Alberto Tejero²; ¹Fossil Ion Technology S.L., Madrid, Spain; ²SEADM, Boecillo, Spain
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- WP 476 **Studies of Dihalogen Radical Anion Formation from Maleic Acid-Acene Compounds by Negative Chemical Ionization (NCI) and Time-of-Flight Mass Spectrometry (TOFMS)**; Daryl Giblin¹; Jonathan P Hopwood²; Brittni A Qualizza²; Jacob W. Cizek²; M. Paul Chiarelli²; Michael L Gross¹; ¹Washington University, St Louis, MO; ²Loyola University, Chicago, IL
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- WP 480 **Ligand Binding Energies and Structural Isomerism Accompanying Phosphine Exchange on the Cationic Gold Clusters;** Marshall Ligare¹; Jose Ulises Reveles²; Grant E Johnson¹; Erin Baker¹; Julia Laskin¹; ¹Pacific Northwest National Lab, Richland, WA; ²Virginia Commonwealth University, Richmond, VA
- WP 481 **Metal Ion Adducts of Cysteine and Cysteine-Containing Peptide Radicals: Structure and Reactivity;** Victor Ryzhov¹; Michael Lesslie¹; John Lawler¹; Kai-Chi Justin Lau²; Alan C Hopkinson²; ¹Northern Illinois University, DeKalb, IL; ²York University, Toronto, Canada
- WP 482 **Mass Spectrometric and Computational Investigation of the Protonated Carnosine-Carboplatin Complex Fragmentation;** Ida Ritacco¹; Emilia Sicilia¹; Tamer Shoeib^{2,3}; Mohamed Korany²; Nino Russo¹; ¹Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Calabria, Italy; ²Department of Chemistry, The American University in Cairo, New Cairo, Egypt; ³Centre for Analytical Science, Department of Chemistry, Loughborough University, Loughborough, UK
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- WP 487 **Determination of Pharmaceuticals in Wastewater using Online SPE Coupled to Liquid Chromatography Mass Spectrometry;** Andreas Bruchmann¹; Claudia vom Eyser²; Thorsten Teutenberg²; Jochen Tuerk²; ¹Axel Semrau GmbH & Co.KG, Sprockhoevel; ²IUTA, Duisburg, Germany
- WP 488 **Applying a Tangential Flow Filtration Approach for Low Concentration Proteomics Sample Preparation;** Woodard Toni¹; Zhe Wang¹; Ma Hongyan¹; Saurav Malla¹; Si Wu¹; ¹University of Oklahoma, Norman, OK
- WP 489 **SPE Method Optimization and Transfer to an Automated Sample Preparation Platform for Low Level Catecholamine Analysis using LC-MS/MS;** Alan Edgington¹; Adam Senior¹; Lee Williams²; Victor Vandell³; Geoff Davies¹; Helen Lodder¹; Rhys Jones¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; Dan Menasco³; ¹Biotage GB Limited, Cardiff, UK; ²Biotage GB Limited, Cardiff; ³Biotage LLC, Charlotte, NC
- WP 490 **Dual Immobilized Enzyme Reactors for Peptide, Glycan, and Glycopeptide online LC-MS/MS Analysis;** Kerry Wooding¹; Rui Zhu¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 491 **Handy Devices for Quantitative Capillary Blood Microsampling;** Shinobu Kudoh¹; Ippei Takeuchi²; ¹Shimadzu Techno-Research, Inc., Ohta-Ku, Tokyo; ²Shimadzu Corp, Kyoto, Japan
- WP 492 **Rapid, Efficient and Reproducible Sample Preparation for Quantitative Proteomics by a Surfactant-Aided Precipitation/On-Pellet Digestion Strategy;** Shichen Shen¹; Bo An¹; Jun Li¹; Xiaomeng Shen¹; Chengjian Tu¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY
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- WP 495 **In-depth Proteomic Quantification of Cell Secretome in Serum-Containing Conditioned Medium;** Yeijing Weng¹; Zhigang Sui¹; Yichu Shan¹; Lihua Zhang¹; Yukui Zhang¹; ¹Chinese Academy of Sciences, Dalian, China
- WP 496 **A Multiwell Magnetic Mixer for Automated Sample Preparation;** Chang Liu¹; Don W Arnold²; Thomas R Covey¹; ¹SCIEX, Concord, ON; ²SCIEX, Redwood City, CA
- WP 497 **Quantitative Analysis of low-Abundance Serological Proteins with Peptide Affinity-Based Enrichment and Pseudo-Multiple Reaction Monitoring by Hybrid Quadrupole Time-Of-Flight Mass Spectrometry;** Kwang Hoe Kim^{1,2}; Yeong Hee Ahn³; Eun Sun Ji¹; Ju Yeon Lee¹; Jin Young Kim¹; Hyun Joo An²; Jong Shin Yoo^{1,2}; ¹Korea Basic Science Institute, Chungbuk, South Korea; ²Chungnam National University, Daejeon, South Korea; ³Cheongju University, Cheongju, South Korea
- WP 498 **Advancing the MStern Blotting – PVDF Membrane-Based Peptide Fractionation in a 96 Well Format;** Sebastian Berger^{1,2}; Saima Ahmed³; Michaela Helmel³; Hanno Steen³; ¹Boston Children's Hospital, Boston, MA; ²Harvard Medical School, Boston, MA; ³Boston Children's Hospital, Harvard Medical School Boston, MA
- WP 499 **Quantification of Celecoxib in Rat Skin using LC-MS/MS Method after Collagenase Digestion and Bead Lysis;** Raghupathi Aleti¹; Ilayaraja Kalaikadhiban¹; Sailakshmi Chennupati¹; Devender Reddy Ajjala¹; Ramakrishna Nirogi¹; ¹Suven Life Sciences Ltd, Hyderabad, Telangana
- WP 500 **Basic Reverse Phase Fractionation on OasisHLB-uElution Plates as a Fast Sample Preparation Technique for LCMSMS Analysis of Low Protein Amounts;** Robert N O'Meally¹; Tatiana N. Boronina¹; Maximilian Konig¹; Felipe Andrade¹; Robert N Cole¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
- WP 501 **LC/MS/MS Analysis with On-line Cartridge for Removal of Phospholipids from Protein Precipitation Biological Fluid Samples;** David S. Bell¹; Xiaoning Lu¹; Hillel K. Brandes¹; Craig R Aurand¹; Sara Smith¹; Carmen T. Santasania¹; ¹MilliporeSigma, Bellefonte, PA
- WP 502 **Different Approach for Improvement of Low Recovery Dried Blood Spot Storage Sample and Its Application in Bioanalytical Assay;** Dawei Zhou¹; John Ma¹; Mohamed Osman¹; Xiping Fang¹; ¹WuXi AppTec Co., Plainsboro, NJ
- WP 503 **Simultaneous Quantitation of Five Leachables in Lipid Emulsions by LC-MS/MS Using 2,2-Dimethoxypropane;** Yousheng Hua¹; Jim Story¹; Peifeng Hu¹; Dennis Jenke¹; Christopher M Jones¹; ¹Baxter Healthcare, Round Lake, IL
- WP 504 **A Conventional Procedure to Reduce Asn Deamidation Artifacts during Trypsin Peptide Mapping;** Yekaterina Kori^{1,2}; Rekha Patel²; Alyssa Neill²; Hongcheng Liu²; ¹University of Massachusetts Amherst, Amherst, MA; ²Alexion Pharmaceuticals, Cheshire, CT

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- WP 506 **Lipidomic Profiling of Biological Samples using Off-Line Two-Dimensional High-Performance Liquid Chromatography-High Resolution Mass Spectrometry**; Monica Narvaez-Rivas¹; Qibin Zhang²; ¹University of North Carolina at Greensboro, Kannapolis, NC; ²University of North Carolina Greensboro, Greensboro, NC
- WP 507 **UHPLC Combined with Ultra-high Resolution QTOF-MS for Rapid Lipidomic Profiling of Serum for Discovery of Lipid Biomarkers of Parkinson's Disease**; Jaspaul Tatlay¹; Dorothea Mung¹; Richard Camicioli²; Liang Li¹; ¹University of Alberta, Edmonton, Canada; ²Neuroscience and Mental Health Institute, Department of Medicine, Edmonton, AB, Canada
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- WP 509 **Comprehensive Lipid and Protein Analysis of Size Fractionated Serum Lipoproteins in Normal versus Dyslipidemic Subjects**; Michael Gardner¹; Zsuzsanna Kuklenyik¹; David M Schieltz¹; Bryan A Parks¹; Jon Rees¹; Lisa G McWilliams¹; Yulanda Williamson¹; Christopher Toth¹; Jeffrey Jones¹; Michael Andrews¹; John R Barr¹; ¹Centers for Disease Control and Prevention, Atlanta, GA
- WP 510 **Reverse Phase LC-ESI-QTOF Methodology for the Analysis of Lipids in Whole Blood**; Ralph Hindle¹; Ken D Stark²; Juan J Aristizabal Henao²; Richard W Smith³; Sheher Mohsin⁴; ¹Vogon Laboratory Services, Alberta, Cochrane, Canada; ²Department of Kinesiology, University of Waterloo, Waterloo ON, Canada; ³University of Waterloo Mass Spectrometry Facility, University of Waterloo, Waterloo ON, Canada; ⁴Agilent Technologies, Schaumburg, IL
- WP 511 **The Application of Lipidomics to the Study of Hepatocellular Carcinoma (HCC) Induced by Low Dose, High-Energy, High Charge Ions (HZE)**; Brooke L Barnette¹; Shinji K Strain¹; Cheryl F Licht¹; Yu Yongjia¹; Robert Ullrich¹; Mark R Emmett¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX
- WP 512 **Analysis of Lipids in Spinal Cords of Experimental Autoimmune Encephalomyelitis (EAE) Mice using On-Line Photochemical Derivatization and Tandem Mass Spectrometry**; Leelyn Chong¹; Xiaoxiao Ma¹; Yu Xia¹; Zheng Ouyang¹; ¹Purdue University, West Lafayette, IN
- WP 513 **Lipid Peroxidation Profiles in Acute Hepatic Ischaemia-Reperfusion Injury**; Michael Dunn¹; Aimen Amer²; Margaret Knight¹; Clair Roper¹; Peter Blain¹; Matthew Wright²; ¹Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK; ²Institute of Cellular Medicine, Newcastle University, Newcastle upon Tyne, UK
- WP 514 **The Comparison of Glycosphingolipids in an Epithelial Ovarian Cancer Cell Line and a Nontumorigenic Epithelial Ovarian Cell Line using MALDI-MS**; Krishani Kumari Rajanayake¹; William Taylor¹; Dragan Isailovic¹; ¹The University of Toledo, Toledo, OH
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- WP 519 **Direct Analysis of Phospholipids in Biological Tissues Using Internal Extractive Electrospray Ionization Mass Spectrometry**; Haiyan Lu¹; Jianyong Zhang²; Wei Zhou³; Yiping Wei²; Huanwen Chen⁴; ¹East china university of Technology, Nanchang, China; ²Second Affiliated Hospital of Nanchang University, Nanchang, China; ³East China Institute of Technology, Nanchang, China; ⁴East China University of Technology, Nanchang, Mainland
- WP 520 **Ambient Ionization Methods and Liquid Chromatography – Mass Spectrometry Analysis of Human Melanoma Biopsies**; Louis Searcy¹; Candice Ulmer²; Matthew Kazaleh²; Michael Costanzo²; Nikolaus Gravenstein²; Richard A. Yost²; ¹University of Florida, Gainesville, FL; ²University of Florida, Gainesville, FL
- WP 521 **In-situ and in-vitro Regional Analysis of Lipids in Mammalian Vitreous Humor using MALDI-MS**; Abby Schnepf¹; M. Cecilia Yappert²; Douglas Borchman³; ¹Department of Chemistry, University of Louisville, Louisville, KY; ²Department of Chemistry University of Louisville, Louisville, KY; ³Department of Ophthalmology and Visual Sciences University of Louisville, Louisville, KY
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- WP 525 **Comprehensive Profiling of Lipids in Chicken Skin by High Resolution Mass Spectrometry with Online Information Dependent Acquisition Workflow**; Yushi Pan¹; Kevin Zhang²; Huaidong Yu³; Yong Fang⁴; ¹Pan YS, Nanjing, China; ²Beijing, Beijing; ³Yu HD, Beijing, China; ⁴Fang Y, Nanjing, China



- WP 526 **Phospholipid Profiling by Two Distinct MRM Measurements to Identify Phospholipid's Class and Fatty Acid Composition;** Tsuyoshi Nakanishi¹; Masaki Yamada¹; Suzumi Tokuoka²; Yoshihiro Kita²; Takao Shimizu^{2,3}; ¹Shimadzu Corporation, Kyoto, Japan; ²The University of Tokyo, Tokyo, Japan; ³National Center for Global Health and Medicine, Tokyo, Japan
- WP 527 **Lipid Profiling of Madin-Darby Canine Kidney Cells and Its Lipid Changes Induced by Aristolochic Acid(I) using Two-Dimensional LC-MS;** Honggang Nie¹; Liu Ranran¹; Yang Youyou²; Liu Huwei¹; Bai Yu¹; ¹Peking University, Beijing, China; ²Chinese Oil & Foodstuffs Corporation (COFCO) Nutrition and Health Research Institute, Beijing, China
- WP 528 **High-Throughput Lipidomics Workflow for Identification and Quantification of >1000 Lipids in 13 Different Lipid Classes;** Richard John Robinson¹; Fred Hubbard¹; Philip Michael Charpia¹; Alexandria Conner¹; Anne Evans²; Luke Miller¹; Steve Watkins¹; Don Harvan¹; ¹Metabolon, Inc., Durham, NC; ²Metabolon, Inc., Durham, NC
- WP 529 **Lipidomic Analysis of Cultured Cells Lines;** Finnur Freyr Eiriksson^{1,2}; Manuela Magnúsdóttir²; Halldorsson Skarphéðinn²; Ottar Rólfsson²; Helga M. Ógmundsdóttir²; Margrét Thorsteinsdóttir^{1,2}; ¹ArcticMass, Reykjavik, Iceland; ²University of Iceland, Reykjavik, Iceland
- WP 530 **Profiling Lipids in Plants Using Infusion and Chromatography Based High Resolution Mass Spectrometry Methods with Automated Data Processing;** Yelena A. Adelfinskaya¹; Daniel J J Gachotte¹; Jeffrey R Gilbert¹; Jesse L Balcer¹; Laura L Wayne¹; ¹Dow AgroSciences, Indianapolis, IN
- WP 531 **Lipid and Fatty Acid Analysis in Grape Seeds and Grape Seed Oil with High Resolution Mass Spectrometry;** Zareen Khan¹; Akanksha Singh²; Ahammed Shabeer T.P.¹; Manoj Pillai³; Kaushik Banerjee¹; ¹National Referral Laboratory, ICAR-National Research Centre for Grapes, Pune, Maharashtra, India; ²SCIEX, Gurgaon, Haryana; ³SCIEX, Gurgaon, Haryana India
- WP 532 **Methods to Analyze Beneath the Surface of Oil Seeds using Mass Spectrometry;** Suresh Annangudi¹; Holly Henderson²; Callee Walsh²; Trust T Razunguzwa²; Jeffrey R Gilbert¹; ¹Dow AgroSciences, Indianapolis, IN; ²Protea Biosciences, Inc. Morgantown, WV
- WP 533 **Accelerating Lipid Profiling Acquisition Strategies using Differential Mobility Spectrometry and SWATH® Data Collection;** Eva Duchoslav¹; Brad T Patterson²; Larry J Campbell¹; Yves J C LeBlanc¹; ¹SCIEX, Concord ON, Canada; ²SCIEX, Melbourne VIC, Australia
- WP 534 **A Simple, Flexible, and Automated Infusion System for Lipidomic Analysis using Mass Spectrometry;** Jeff McDonald¹; Steve Stiller²; ¹UT Southwestern Medical Center, Dallas, TX; ²LEAP Technologies, Carrboro, NC
- WP 535 **The Rapid Evaporative Ionisation Mass Spectrometry (REIMS) iKnife Identifies Gynaecological Tissue with Excellent Accuracy in the ex-vivo and in-vivo Setting;** David L Phelps¹; Julia Balog^{1,2}; Louise Gildea¹; Mona El-Bahrawy¹; Abigail Speller¹; Robert Brown¹; Sadaf Ghaem-Maghani¹; Zoltan Takats³; ¹Imperial College, London, UK; ²Waters Corporation, Budapest, Hungary; ³Imperial College London, South Kensington Campus London, UK
- WP 536 **REIMS has the Potential to Improve Diagnostic of Hepatocellular Carcinoma Liver – Perspectives towards Intraoperative Molecular Diagnostics;** Tiffany Porta¹; Julia Balog²; Flora Olivier¹; Pierre-Maxence Vaysse¹; Ulf P. Neumann³; Steven W.M. Olde Damink⁴; Thorsten Cramer³; Ron M.A. Heeren¹; ¹M4I Institute - Maastricht University, Maastricht, The Netherlands; ²Waters Corporation, Wilmslow, UK; ³RWTH Aachen, Aachen, Germany; ⁴Maastricht University Medical Center +, Maastricht, The Netherlands

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- WP 538 **Integrative Pathway Analysis of Metabolic Signature in Bladder Cancer: A Linkage to Cancer Genome Atlas Project and Prediction of Survival;** Nagireddy Putluri; Baylor College of Medicine, Houston, TX
- WP 539 **Development of Highly Sensitive Quantification Method for Testosterone Human Serum by Liquid Chromatography–Tandem Mass Spectrometry;** Vasanta Putluri¹; Sriramy Donepudi¹; Feng Jin¹; Andre Szczesniowski²; Vadiraja B Bhat²; J Peter Cook¹; Dolores J Lamb¹; Arun Sreekumar¹; Nagireddy Putluri¹; ¹Baylor College of Medicine, Houston, TX; ²Agilent Technologies, Wilmington, DE
- WP 540 **Targeted Metabolomics of Liver Donor Allografts: A Clinical Application;** Jeffrey A Culver^{1,2}; Andrew V Zelenin^{1,2}; Christopher Petucci^{1,2}; Stephen J Gardell^{1,2}; John B Seal³; ¹Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; ²Southeast Center For Integrated Metabolomics, Gainesville, FL; ³Ochsner Medical Center, New Orleans, LA
- WP 541 **Metabolomics and Flux Analysis Informed on the Mechanism of Response of AML to IACS-10759, a Potent and Selective OXPHOS Inhibitor;** Pietro Morlacchi; UT MD Anderson Cancer Center (IACS/CCCT), Houston, TX
- WP 542 **Use of a Novel C18-Based Stationary Phase for Human Urine Metabolite Profiling By UHPLC-High Resolution Accurate Mass Spectrometry (HRAM);** Alan P McKeown¹; Catherine Otori²; Geoffrey Faden³; ¹Advanced Chromatography Technologies Ltd, Aberdeen; ²The School of Pharmacy, University of Nottingham, Nottingham, UK; ³MACMOD Analytical Inc., Chadds Ford, PA
- WP 543 **Discriminatory Ability of Ambient Ionisation Mass Spectrometry in Analysing Skin Secretions: A Non-Invasive Diagnostic Test of Lower Airway Infection;** Emmanuelle Bardin¹; Frances Bolt¹; Eric Alton^{1,2}; Andrew Bush^{1,2}; Jane Davies^{1,2}; Zoltan Takats¹; ¹Imperial College London, South Kensington Campus London, UK; ²Royal Brompton and Harefield NHS Foundation Trust, London, UK
- WP 544 **Comprehensive Cerebrospinal Fluid Metabolomic Profiling for Mechanism Study of Idiopathic Intracranial Hypertension;** Liang Zhao¹; Xiali Zhong¹; Abhay Moghekar¹; Thomas Hartung¹; ¹Johns Hopkins University, Baltimore, MD
- WP 545 **Isotope-based Metabolomic Analysis of Human Samples;** Kevin Y Cho¹; Ying-Jr Amanda Chen¹; Nathaniel G Mahieu¹; Gary Patti¹; ¹Washington University School of Medicine, St. Louis, MO
- WP 546 **Integrative Metabolomic and Proteomic Analysis Reveals Biomarkers Related to Oxidative Stress in Traumatic Brain Injury;** Veera Venkata Ratnam Bandaru¹; Sartaj Ahmad Mir¹; Frederick Korley¹; Robert D Stevens¹; Akhilesh Pandey¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
- WP 547 **Bioaccessible Phytochemicals from Black Raspberries after Interaction with Saliva – Determining Exposure in the Oral Cavity Using a Metabolomics Approach;** Ken M Riedl¹; Jennifer Ahn-Jarvis¹; Matthew Teegarden¹; Thomas Knobloch¹; Christopher Weghorst¹; Purnima Kumar¹; Steven Clinton¹; Yael Vodovotz¹; Steven J Schwartz¹; ¹The Ohio State University, Columbus, OH

- WP 548 **Studying Individual Differences in Cancer Drug Efficacy using Metabolomics of a Panel of Human Cell Lines;** Thomas Hankemeier¹; Liewei Wang²; Ruud Berger³; Amy Harms³; Slavik Koval³; Sabine Bos³; Silvia Marin⁴; Marta Cascante⁴; Dick Weinshilboum⁵; Rima Kaddurah-Daouk⁶; ¹Leiden University, Leiden, South Holland; ²Clinical Pharmacology, Mayo Clinic, Rochester, MN; ³Leiden University, Leiden, Netherlands; ⁴University of Barcelona (UB); ⁵Mayo Clinic, Rochester, MN; ⁶Duke University Medical Center, Durham, NC
- WP 549 **Lipidomic Analysis of Endometriosis Foci by Direct Tissue-Spray Mass Spectrometry;** Vitaliy Chagovets¹; Zhihao Wang²; Anna Borisova¹; Vadim Lagutin¹; Natalia Starodubtseva¹; Andrey Kozachenko¹; Konstantin Chingin²; Chen Huanwen²; Leila V Adamyan¹; Vladimir Frankevich¹; Gennady Sukhikh¹; ¹Research Center for Obstetrics, Gynecology and Perinatology of the Ministry of Healthcare of the Russian Federation, Moscow; ²Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China University of Technology, Nanchang, China
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- WP 550 **Drosophila as a Model System for Microbiome Research - a GCMS Based Metabolomics Approach;** Bhavapriya Vaitheesvaran¹; John McMullen²; Anthony Macherone³; Angela E Douglas²; Justin R Cross¹; ¹Memorial Sloan Kettering Cancer Center, New York, NY; ²Cornell University, Ithaca, NY; ³Agilent Technologies, Little Falls, DE
- WP 551 **Lipidome and Metabolome Analyses of Mouse Hippocampus in Response to Low-dose X-ray Irradiation using Liquid Chromatography-Mass Spectrometry;** Fereshteh Zandkarimi¹; Jeffrey Morré¹; Jacob Raber²; Claudia S Maier¹; ¹Oregon State University, Department of Chemistry Corvallis, OR; ²OHSU, Dep. Behavioral Neuroscience, Neurology, & Radiation Medicine, ONPRC, Portland, OR
- WP 552 **Comparative High Resolution Metabolomics of Metastatic vs. Non-Metastatic Tumors in a Murine Medulloblastoma Model;** Danning Huang¹; Martin R L Paine¹; Jingbo Liu²; Sophia Banton²; Shuzhao Li²; Tobey MacDonald²; Facundo M Fernández¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Emory University School of Medicine, Atlanta, GA
- WP 553 **Caloric Restriction Improves Diabetes-Induced Nonalcoholic Fatty Liver Diseases by Changing Metabolism;** Youngae Jung¹; Geum-Sook Hwang^{1,2}; ¹Western Seoul Center, Korea Basic Science Institute, Seoul, Republic of Korea; ²Department of Life Science, Ewha Womans University, Seoul, Republic of Korea
- WP 554 **Comprehensive HPLC-MS Metabolomics Analysis of Brain Tissue Reveals Age, Region, and Gender-Specific Effects of *Centella asiatica*;** Parnian Lak¹; Nora Gray²; Luisa Zini³; Phillip Seitzer³; Christopher Harris²; Joseph Quinn^{2,4,5}; Amala Soumyanath²; Jan Fred Stevens¹; Claudia Maier¹; ¹Oregon State University, Corvallis, OR; ²Oregon Health and Sciences University, Portland, OR; ³Proteome Software, Portland, OR; ⁴PADRECC, Portland, OR; ⁵Portland Veterans Affairs Medical Center, Portland, OR
- WP 555 **Global Lipid Profiling in Aging Mouse Model associated with Osteoporosis;** Eun-ha Kim¹; Geum-Sook Hwang¹; ¹KBSI Western Seoul Center, Seoul, Republic of Korea
- WP 556 **Metabolomics Approach for Mice Serum Associated with Epidermal Growth Factor Receptor and BaP-induced Mouse Lung Tumor Genesis using Liquid Chroma;** Hui Ling Lee; *Fu Jen Catholic University, New Taipei, TAIWAN*
- WP 557 **Global Metabolomic Profile Differentially Segregates with Calcium Supplementation in Mice Fed a High-Fat Western Style Diet;** Muhammad Aslam¹; Li Zhang²; Christine Bassis¹; Maureen Kachman²; Charles Burant²; Ingrid Bergin³; James Varani¹; ¹Department of Pathology, Internal Medicine, Medical of School, University of Michigan, Ann Arbor, MI; ²Michigan Regional Comprehensive Metabolomics Resource Center; University of Michigan, Ann Arbor, MI; ³Unit for Laboratory Animal Medicine, University of Michigan, Ann Arbor, MI
- WP 558 **LC-MS/MS Based Metabolomic Analysis of the Effect of Biogenic Amine in a LPS-induced Sepsis Mouse Model;** Yu-Min Liu¹; Soo-Ray Wang²; Maw-Rong Lee¹; ¹National Chung-Hsing University, Taichung, Taiwan (R.O.C.); ²Chung Shan Medical University, Taichung, Taiwan (R.O.C.)
- WP 559 **Diabetes Markers: Using Orbitrap HRAM and a New Workflow for Differential Analysis of Zucker Rat Plasma Metabolome;** Junhua Wang¹; Maciej P Bromirski²; Ralf Tautenhahn³; David Peake⁴; Kiyonami Reiko⁴; Tina Settineri⁴; Ken Miller⁴; ¹Thermo Fisher Scientific Inc, San Jose, CA; ²Thermo Fisher Scientific, Bremen, DE; ³Thermo Fisher Scientific, San Jose, CA; ⁴ThermoFisher, San Jose, CA
- WP 560 **Effects of Dietary Different Doses of Copper and High Fructose Feeding on Rat Fecal Metabolome;** Biyun Shi^{1,2}; Ming Song³; Xiaoli Wei^{1,2}; Xinmin Yin^{1,2}; Dale Schuschke⁴; Imhoi Koo^{1,2}; Craig McClain^{3,5}; Xiang Zhang^{1,2,5}; ¹Department of Chemistry, University of Louisville, Louisville, KY; ²Center for Regulatory and Environmental Analytical Metabolomics, University of Louisville, Louisville, KY; ³Department of Medicine, University of Louisville, Louisville, KY; ⁴Department of Physiology and Biophysics, University of Louisville, Louisville, KY; ⁵Department of Pharmacology and Toxicology, University of Louisville, Louisville, KY
- WP 561 **Optimization of Tissue Extraction for GCMS Metabolomic Analysis Reveals Altered Metabolism of Barbiturates in a Polycystic Kidney Disease Model;** Hayley Abbiss^{1,2,3}; Garth L. Maker^{3,4,5}; Gabrielle C. Musk^{4,6}; Catherine Rawlinson^{3,4,5,7}; Joel P.A. Gummer^{3,4}; Patricia A. Fleming⁴; Jacqueline K. Phillips⁸; Mary C. Boyce⁹; John Moncur²; Robert D. Trengove^{3,4,5}; ¹Murdoch University, Perth, Western Australia; ²SpectralWorks, Cheshire, UK; ³Separation Science and Metabolomics Laboratory, Perth, Australia; ⁴Murdoch University, Perth, Australia; ⁵Metabolomics Australia, Western Australian Node, Perth, Australia; ⁶The University of Western Australia, Perth, Australia; ⁷Curtin University, Perth, Australia; ⁸Macquarie University, Sydney, Australia; ⁹Edith Cowan University, Perth, Australia
- WP 562 **Spatial-temporal Analysis of Metabolite Expression in *Xenopus laevis* embryos during Early Development;** Jennifer Arceo¹; Nicole M Schiavone²; Danielle A Boley²; Norman J Dovichi²; ¹University of Notre Dame, Notre Dame, IN; ²University of Notre Dame, Notre Dame, IN
- WP 563 **Capillary Zone Electrophoresis-Electrospray Ionization-Mass Spectrometry for *Xenopus laevis* metabolomic Analysis;** Nicole Schiavone¹; Jennifer Arceo¹; Danielle A Boley¹; Norman J Dovichi¹; ¹University of Notre Dame, Notre Dame, IN
- WP 564 **Evaluating the Metabolic Impact of Feeding Baboons a High Fat, High Caloric Diet using an Accurate Mass GC/QTOF;** Mark Libardoni¹; Matthew Curtis²; Stephan Baumann²; ¹Southwest Research Institute, San Antonio, TX; ²Agilent Technologies, Santa Clara, CA
- WP 565 **Profiling and Quantitative Analysis of Small Molecule Metabolites and Neurotransmitters in Crustacean Hemolymph/Neuronal Tissues Using Reversed-Phase and Mix-Mode LC-MS/MS;** Qinjingwen Cao¹; Chuanzi OuYang¹; Xuefei Zhong²; Lingjun Li^{1,2}; ¹University of



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- Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- WP 566 **An Untargeted Metabolomics Approach for Determining Biomarkers Involved in Spontaneous Pre-Term Birth (sp-PTB) Delivery, using a Label-Free LC-DIA-MS Approach;** Shirish Yakkundi¹; Lee Gethings²; James Langridge²; Louise Kenny^{3,4}; ¹Cork University Maternity Hospital, Cork; ²Waters, Wilmslow, UK; ³Cork University Maternity Hospital, Cork, Ireland; ⁴University College Cork, Cork, Ireland
- WP 567 **Global Metabolomics and Lipidomics of Non-Alcoholic Fatty Liver Disease and Non-Alcoholic Steatohepatitis in Human Plasma by LC-HRMS;** Allison J Levy¹; Rainey E Patterson¹; Jeremy P Koelmel¹; Srilaxmi Kalavalapalli²; Nishanth Sunny²; Fernando Brill²; Kenneth Cusi²; Timothy J Garrett³; Richard A Yost^{1,3}; ¹Chemistry Department, University of Florida, Gainesville, FL; ²Department of Medicine, University of Florida, Gainesville, FL; ³Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL
- WP 568 **Comparative Evaluation of Open Access Software used in Liquid Chromatography-Mass Spectrometry Based Untargeted Metabolomics;** Stephanie Samra¹; Benjamin Wancewicz¹; Brian DeFelice¹; Oliver Fiehn¹; ¹UC Davis, Davis, CA
- WP 569 **IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts;** Lee A Gethings¹; Johannes PC Vissers¹; Jose Castro-Perez²; Yvonne Woolerton³; Lynn McLean³; Robert Beynon³; James I Langridge¹; ¹Waters, Wilmslow, UK; ²Waters Corp., Milford, MA; ³Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK
- WP 570 **Evaluation of Ion Mobility/ TOF Mass Spectrometry with Multiple LC Method Parameters for Enhanced Detection in Metabolic Profiling;** Paul Rainville¹; David Heywood¹; Langridge James²; Robert Plumb¹; Jose Castro-Perez¹; ¹Waters, Milford, MA; ²Waters, Manchester, UK
- WP 571 **Profiling the Gut Microbiota Metabolome using HPLC coupled to Ion Mobility-Mass Spectrometry to Study Obesity;** James Poland¹; Alexandra C Schrimpe-Rutledge¹; Charles Robb Flynn²; John A McLean¹; ¹Vanderbilt Dept. of Chemistry, Nashville, TN; ²Vanderbilt University, Nashville TN USA Nashville, TN
- WP 572 **Identification of Eicosanoids Mediating Thromboresistance using an Untargeted Metabolomics and Informatics Approach;** Patrizia B Stadler¹; Shunyan Mo¹; Phillip Seitzer²; Christopher M Colangelo³; Jeffrey J Rade¹; Scott A Shaffer¹; ¹University of Massachusetts Medical School, Worcester, MA; ²Proteome Software, Portland, OR; ³Primary Ion, Old Lyme, CT
- WP 573 **Untargeted Profiling using GC-QTOF MS and Parallel EI and CI analysis to Identify Biomarker Panels to Stratify Patients for Treatment;** Robert Trengove^{1,2,3}; Tom Dignan^{2,4}; Ben Hunter^{2,4}; Garth Maker^{2,4}; Hayley Abbiss^{2,4}; Joel Gummer^{2,3,4}; ¹Murdoch University, Murdoch, WA; ²Separation Science and Metabolomics Laboratory, Perth, Australia; ³Metabolomics Australia, WA Node, Murdoch, Australia; ⁴School of Veterinary and Life Sciences, Murdoch University, Murdoch, Australia
- WP 574 **Metabolomic Analysis of Melanoma Skin Tissues by Liquid Chromatography – Mass Spectrometry;** Matthew Kazaleh¹; Candice Ulmer¹; Louis Searcy¹; Michael Costanzo¹; Nikolaus Gravenstein¹; Richard A Yost¹; ¹University of Florida, Gainesville, FL
- WP 575 **Segmented Flow Sampling with Push-Pull Theta Pipettes for Electrospray Ionization Mass Spectrometry;** Anumita Saha-Shah¹; Curtis M Green¹; David H Abraham¹; Lane A Baker¹; ¹Indiana University Dept. Chemistry, Bloomington, IN
- WP 576 **Development of a Microfluidic Platform for High Throughput Validation of Candidate Disease Biomarkers;** I-Hsuan Chen¹; Ning Bao²; Weiguo Andy Tao¹; ¹Purdue University, West Lafayette, IN; ²Nantong University, Nantong, China
- WP 577 **Ionic Liquid Matrices for MALDI Analysis and CE Separation;** Leila Josefsson¹; Johan Jacksen¹; Åsa Emmer¹; ¹KTH Royal Institute of Technology, Stockholm, Sweden
- WP 578 **Sensitivity Gains using Microflow LC/MS for Oligonucleotide Analysis;** Michael Donegan¹; James P Murphy¹; ¹Waters, Milford, MA
- WP 579 **Study of Ionization Efficiency on Silicon-Based, Micro-Fabricated Electrospray Nozzles for Micro Flow LC-ESI-MS applications;** Christine Wang¹; Simon J Prosser¹; Jamey Jones¹; Daniel Eikel¹; ¹Advion, Inc. Ithaca, NY
- WP 580 **Decreasing Cycle Time While Maintaining Analytical Sensitivity in Microflow LC/MS utilizing a Novel Valve Switching Algorithm;** Jay S. Johnson¹; James P Murphy²; ¹Water Corporation, Milford, MA; ²Waters Corporation, Milford, MA
- WP 581 **Post-column Addition as a Tool to Enhance Performance in Microflow LC/MS;** Angela Doneanu¹; Catherine Tremblay¹; Michael P Donegan¹; James P Murphy¹; ¹Waters, Milford, MA
- WP 582 **Increasing Operable Flow Range of a Nano-spray Source for High-Performance Microspray on a Curtain Gas Equipped Triple –Quadrupole API-MS;** Amanda Berg¹; Helena Svobodova²; Gary A Valaskovic²; ¹New Objective, Inc., Woburn, MA; ²New Objective, Woburn, MA
- WP 583 **Picodroplet Mass Spectrometry for Miniaturized High Throughput Analysis of Synthetic Biology Clones;** Xin Li¹; Murray J Brown²; Clive A Smith¹; Gareth R Cooper²; Xin Liu¹; Anthony Dossang²; Marian Rehak¹; Angela Bridges²; Vinayaka Pawate¹; Bill J Leavens²; ¹Sphere Fluidics Limited, The Jonas Webb Building, Babraham Research Campus, Cambridge, UK; ²GSK Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire, UK
- WP 584 **High-throughput Enzymatic Characterization by Integration of Nanostructure-Initiator Mass Spectrometry and Droplet to Digital (D2D) Microfluidics;** Joshua Vance Heinemann¹; Kai Deng^{2,3}; Steve C.C. Shih²; Jian Gao¹; Markus de Raad¹; Benjamin P Bowen^{1,3}; Paul D Adams^{1,3}; Anup K. Singh^{2,3}; Trent Northen^{1,3}; ¹Lawrence Berkeley Nat'l Lab, Berkeley, CA; ²Sandia National Laboratories, Albuquerque, NM; ³Joint BioEnergy Institute, Emeryville, CA
- WP 585 **A Novel Targeted Metabolic Profiling Workflow for Simultaneous Reverse Phase and HILIC microflow LC-MS/MS Analysis;** Daniel M Warren¹; Jeffery D Miller¹; ¹SCIEX, Redwood City, CA
- WP 586 **An Affordable and Simple-To-Use Snap-Chip-iMALDI Technology for Measuring Plasma Rennin Activity;** Huiyan Li^{1,2,3}; Arya Tavakoli^{2,3}; Robert Popp¹; Christoph H. Borchers^{4,5}; David Juncker^{2,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Biomedical Engineering Department, McGill University, Montreal, QC, Canada; ³McGill University and Genome Quebec Innovation Centre, Montreal, QC, Canada; ⁴University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁵Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

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- WP 587 **Quantitative Analysis of Crosslinked Protein Complexes: A Novel Interactome Approach to Assess Pathogen-Triggered Unconventional Secretion in Arabidopsis**; Tricia Ho¹; Kevin Blackburn¹; John D Williamson¹; Michael B Goshe¹; ¹North Carolina State University, Raleigh, NC
- WP 588 **Identification of Direct Substrates of MAP Kinases Activated by Environmental Stresses in Arabidopsis Thaliana through Protein Kinase Assay Linked-Phosphoproteomics**; Chuan-Chih Hsu¹; Pengcheng Wang²; Chunzhao Zhao²; Jian-kang Zhu²; Weiguo Andy Tao²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN
- WP 589 **Chloroplast Protein Maturation, Regulation and Degradation**; Elden E. Rowland¹; Jitae Kim¹; Klaas J. van Wijk¹; ¹Cornell University, Ithaca, NY
- WP 590 **Emerging Role of Sirtuins and Lysine Acylation in the Regulation of Plant Metabolism**; Dana M Freund¹; Jerry D Cohen¹; Adrian D. Hegeman¹; ¹University of Minnesota at Twin Cities, Saint Paul, MN
- WP 591 **Label-free Quantitative Mass Spectrometry-Based Proteomic Approach for Comprehensive Analysis of Protein Complexes and Protein-Protein Interactions in Plants**; Uma Aryal¹; Zachary McBride²; Donglai Chen²; Jun Xie²; Daniel Szymanski²; ¹Purdue Proteomics Facility, Bindley Bioscience Center, West Lafayette, IN; ²Purdue University, West Lafayette, IN
- WP 592 **Plant Proteomes Aplenty: Quantitative and Phylogenetic Analysis of Five Angiosperms, a Gymnosperm and a Bryophyte**; Harald Marx¹; Alicia L Richards¹; Dhileepkumar Jayaraman¹; Jean-Michel Ané¹; Joshua J Coon¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 593 **Investigating the Expressed Kinome in *C. reinhardtii***; Emily Werth¹; T.S. Karim Gilbert²; Lee M Graves²; Leslie M Hicks¹; ¹UNC Chapel Hill, Department of Chemistry Chapel Hill, NC; ²UNC Chapel Hill, School of Medicine Chapel Hill, NC
- WP 594 **Quantitative Proteomics of Phaeodactylum tricornutum in Phosphate Limited Environment**; Shiang-Yu Tsai¹; Pang-Hung Hsu¹; ¹Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan
- WP 595 **UHPLC-HRMS Analysis of Herbal Plant Extracts to Screen for Small Molecule Drugs with Antibacterial Activity**; Gaganpreet Monga¹; Anima Ghosal¹; Dil Ramanathan¹; ¹Kean University, Union, NJ
- WP 596 **Comparative Protein Analysis of Oil Palm Mesocarp from *Elaeis guineensis* and *Elaeis oleifera* to Investigate Acidification Process**; Jessica K. A. Macêdo¹; Jorge C. Rodrigues-Neto^{1,2}; Jéssica S. Barros^{1,3}; Letícia Jungmann¹; Patrícia Verardi Abdelnur⁴; ¹Embrapa Agroenergy, Brasília, Brazil; ²Federal University of Goiás, Goiânia, Brazil; ³University of Brasília, Brasília, Brazil; ⁴Embrapa Agroenergy, Brasília, DF
- WP 597 **MALDI-Mass Spectrometric Imaging of Endogenous Peptides and Proteins in *Medicago truncatula***; Caitlin Keller¹; Erin Gemperline¹; Junko Maeda¹; Dhileepkumar Jayaraman¹; Michael R Sussman¹; Jean-Michel Ané¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 598 **iTRAQ 8-plex Labeling-Based Proteomics Analysis Reveals Difference of Protein Expression from Sorghum Root which was Treated by Aluminum**; Yong Yang; USDA-ARS at Cornell University, Ithaca, NY
- WP 599 **Extracellular Proteomic Response of Thermally Stressed *Symbiodinium*: Implications for Symbiosis Breakdown during Bleaching**; Contessa Ricci¹; Bren Ledbetter¹; Tam Nguyen¹; Saiful M Chowdhury¹; Laura Mydlarz¹; ¹University of Texas at Arlington, Arlington, TX
- WP 600 **Deep Proteome Analysis of Gerontoplasts from the Inner Integument of Developing Seeds of *Jatropha curcas***; Mohibullah Shah¹; Emanuela L. Soares¹; Magda alberto fernandez lima¹; Camila B. Pinheiro¹; Arlete A. Soares¹; Gilberto B Domont²; Fabio CS Nogueira³; Francisco A. P. Campos¹; ¹Federal University of Ceará, Fortaleza, Brazil; ²Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; ³UFRJ, Rio de Janeiro, Rio de Janeiro
- WP 601 **Quantitative Proteomics of *Phaeodactylum tricornutum* in Acidified Environment**; Tai-Yi Jiang¹; Pang-Hung Hsu¹; ¹Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan
- WP 602 **Standard-flow UHPLC Coupled with TripleQuad MS is a Versatile Platform for Both Targeted Metabolomics and Proteomics**; Daniel Vik¹; Meike Burrow²; Barbara Ann Halkier²; ¹University of Copenhagen, Frederiksberg C, Denmark; ²University of Copenhagen, Copenhagen, Denmark
- WP 603 **Stable Isotopic Labeling of Intact Plants for Molecular Turnover Measurement by HRMS: New Labeling Apparatus and Data Processing Approaches**; Calvin P Peters¹; Dana M Freund¹; Aaron K Rendahl¹; Jerry D Cohen¹; Adrian D. Hegeman¹; ¹University of Minnesota at Twin Cities, Saint Paul, MN
- WP 604 **Multi-OMICS Investigation of the Lignin Deposition Altering Enzyme Family of Arogonate Dehydratases in Arabidopsis and Poplar Tree**; Kim K. Hixson; Washington State University, Richland, WA
- WP 605 **Qualification and Quantification of Cannabinoids and Terpenes in Extracts of Cannabis sativa by Gas Chromatography – Mass Spectrometry**; Allegra Leghissa¹; Zacariah L. Hildenbrand²; Sean Jun³; Aaron L Hicks³; Kevin A Schug¹; ¹The University of Texas at Arlington, Arlington, TX; ²Inform Environmental, LLC, Dallas, TX; ³C4 Laboratories, LLC, Mesa, AZ
- WP 606 **Systemic Defense Induction and Post-Ingestive Rearrangement of Plant Toxins in Insects – a Metabolomics Approach Driven by Automated Compound Identification**; Sven Heiling¹; Aiko Barsch²; Heiko Neuweiger³; Emmanuel Gaquerel⁴; Ian T Baldwin⁵; ¹Max-Planck-Society, Jena, Thüringen; ²Bruker Daltonics Ltd, Bremen, DE; ³Bruker Daltonics Ltd, Bremen, Germany; ⁴Centre for Organismal Studies Heidelberg, Heidelberg, DE; ⁵Max Planck Institute for Chemical Ecology, Jena, DE
- WP 607 **Metabolic Profiling of Stilbenes by LC-MS for Genetic Analysis in an F2 Interspecific Grapevine Hybrid Family**; Soon Li Teh¹; Bety Rostandy¹; Mani Awale²; Shanshan Yang³; Jonathan Fresno-Ramirez³; Qi Sun³; Matthew D. Clark¹; Anne Y. Fennell²; James J. Luby¹; Adrian D. Hegeman¹; ¹University of Minnesota at Twin Cities, Saint Paul, MN; ²South Dakota State University, Brookings, SD; ³Cornell University, Ithaca, NY
- WP 608 **Comprehensive Analysis of Tropical Flower Secondary Metabolites**; Elena Stashenko; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia
- WP 609 **Accounting for Complexity: A Procedure for the Targeted Analysis of Primary- and Secondary-Metabolites, and Phytohormones from a Single Plant Extract**; Martin Schäfer¹; Christoph Brütting¹; Mario Kallenbach¹; Gordon van 't Slot²; Paul Speir³; Ian T Baldwin¹; ¹Max Planck Institute for Chemical Ecology, Department of Molecular Ecology, Jena, Germany; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics, Inc., Billerica, MA
- WP 610 **Depth Profiling of Whole Soybean Nodules using Laser Ablation Electrospray Ionization Mass Spectrometry**; Christopher Anderton¹; Sylwia A Stopka²; Beverly J Agtuca³; Rosalie K Chu¹; David W Koppenaal¹; Gary Stacey³; Akos Vertes²; Ljiljana Pasa-Tolic¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²George Washington University, Washington DC; ³University of Missouri, Columbia, MO

- WP 611 **Identificación of Metabolites Involved in the Color Reversion Process in Blackberry Fruit using LC-ESI-QTOF**; Victor Manuel Mondragon Olguin¹; Georgina Alejandra Pérez Pérez²; Edmundo M. Mercado Silva²; Gelasio Perez¹; ¹Agilent Technologies Mexico, Mexico, DF; ²Universidad Autonoma de Queretaro, Queretaro, QRO
- WP 612 **REIMS (Rapid Evaporative Ionization Mass Spectrometry) and Multi-Variant Statistics, Two Tools in Support of Weed Grass Speciation and Phenotype Characterization**; Sara Stead¹; Jackson Pope²; Robert Edwards³; Melissa Brazier-Hicks³; Catherine Tetard-Jones³; Zoltan Takats⁴; ¹Waters corp, Manchester, Lanc; ²Waters, Wilmslow, UK; ³University of Newcastle, Newcastle upon Tyne, UK; ⁴Imperial College, London, UK
- WP 613 **DESI-MS Imaging with Ion Mobility and Multivariate Analysis for the Determination of Weed Grass Species and Surface Level Characteristics**; Philippa Jayne Hart¹; Sara Stead¹; Emmanuelle Claude¹; Hernando Olivos²; Melissa Brazier-Hicks³; Catherine Tetard-Jones³; Robert Edwards³; ¹Waters Corporation, Wilmslow, UK; ²Waters Corporation, Beverly, Massachusetts; ³Newcastle University, Newcastle upon Tyne, UK
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- WP 614 **Method Development of an Automated Hybrid LBA-LC/MS Assay for the Quantitative Bioanalysis of the Biotherapeutic Teriparatide in Human Plasma**; Jean-Nicholas Mess¹; Daniel Villeneuve¹; Georges Koudssi¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- WP 615 **Improving the Sensitivity for an Immunocapture LC-MS Assay of Infliximab in Rat Plasma Using Trap-and-Elute MicroLC-MS**; Remco van Soest¹; Lei Xiong¹; ¹SCIEX, Redwood City, CA
- WP 616 **Development and Validation of an LC-MS/MS Method for the Quantitation of Linker-extended Cyanovirin-N in Rat Plasma**; Hui Hong¹; Wenzhong Liang¹; Xin Zhang¹; Xinping Fang¹; ¹WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China
- WP 617 **Quantitation of Insulin Glargine and Major Metabolites in Human Plasma Using Hybrid LBA-LC/MS with Automated Magnetic Particle Processing**; Kevork Mekhssian¹; Jean-Nicholas Mess¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- WP 618 **Quantitation of a Modified Insulin in Rat Plasma Using Triple Quad 6500 LC-MS/MS**; Rong Huang¹; Guangchun Zhou¹; Joshua Froning¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- WP 619 **Automated Biotherapeutic Quantitation from Tissue**; Kristin Geddes¹; Lisa A Vasicek²; Daniel S Spellman²; Kevin P Bateman²; ¹Merck and Co, Inc, West Point, PA; ²Merck & Co., Inc., West Point, PA
- WP 620 **Quantitative Bioanalysis of Rituximab and Reditux for Biosimilarity Assessment Comparing Triple Quadrupole and Hybrid Time-of-Flight Platforms**; Richard Lavallée¹; Daniel Villeneuve¹; Kevork Mekhssian¹; Jean-Nicholas Mess¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- WP 621 **Using a Tandem Protein Precipitation/Immunoaffinity Purification Extraction to Resolve Specificity and Sensitivity Roadblocks: Bioanalysis of a PEGylated Human Protein Analog**; Jonathan R St-Germain¹; Luca Genovesi¹; Jean-Nicholas Mess¹; Anthony T Murphy²; Selina Estwick²; Patricia L Brown-Augsburger²; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada; ²Eli Lilly and Company, Indianapolis, IN
- WP 622 **Comparison of Bottom-Up and Top-Down Analytical Methodologies for the Quantitative Bioanalysis of Large Therapeutic Peptides in Biological Matrix**; Georges Koudssi¹; Jean-Nicholas Mess¹; Anahita Keyhani¹; ¹Algorithme Pharma Inc., Laval, Canada
- WP 623 **Generic Quantitative LC-MS/MS Assay for Analysis of hlgG1 Based Therapeutic Proteins in Cynomolgus Monkey Serum Using Immunocapture with MSIA™-D.A.R.T.'S™**; Christian Lanshoeft^{1,2}; Olivier Heudi¹; Sarah Cianféran²; Eric E Niederkofer³; Ravindra Chaudhari³; Andrew Paul Warren¹; Franck Picard¹; Olivier Kretz¹; ¹Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; ²Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; ³Thermo Fisher Scientific, Tempe, AZ
- WP 624 **Applying Rapid Trypsin Digestion for Targeted Protein Quantitation in Rat Plasma by Liquid Chromatography/Tandem Mass Spectrometry**; Moucun Yuan¹; Morse Faria¹; Jinlin Shen¹; Song Zhao¹; Eric Ma¹; Elizabeth Dompkowski¹; Michael Waldron¹; Bruce Hidy¹; William R. Mylott Jr. ¹; Rand Jenkins¹; ¹PPD, Richmond, VA
- WP 625 **Absolute Quantitation of Glycan and Site-Specific Glycoforms on Commercial mAbs using Multiple Reaction Monitoring**; Nari Seo¹; Unyong Kim²; Hyun Joo An¹; ¹GRAS&AGRS, Chungnam National University, Daejeon, Republic of Korea; ²Asia-Pacific Glycomics Reference Site (AGRS), Daejeon, Republic of Korea
- WP 626 **Improved Reagents and Software for Comparing Biosimilar and Originator Therapeutic Proteins: Accurate Analysis of Deamidation and Disulfide Bond Scrambling**; Wilfred H Tang¹; Marshall Bern¹; John St Skilton¹; Eric Carlson¹; Michael J Ford²; Karthik Pisupati³; Anna Schwendeman³; Chris Hosfield⁴; Sergei Saveliev⁴; Michael M Rosenblatt⁴; Marjeta Urh⁴; Chris Becker¹; ¹Protein Metrics Inc., San Carlos, CA; ²MS Bioworks, LLC Ann Arbor, MI; ³University of Michigan, Ann Arbor, MI; ⁴Promega Corp, Madison, WI
- WP 627 **The Use of Generic Surrogate Peptides for the Quantitative Analysis of hlgG1 in Pre-Clinical Species with High-Resolution Mass Spectrometry**; Christian Lanshoeft^{1,2}; Thierry Wolf¹; Olivier Heudi¹; Sarah Cianféran²; Samuel Barteau¹; Markus Walles¹; Kelly B Doering³; Guillaume Bechade⁴; Franck Picard¹; Olivier Kretz¹; ¹Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; ²Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; ³Waters, Milford, MA; ⁴Waters AG, Baden-Daettwil, Switzerland
- WP 628 **Host Cell Protein Analysis by microflow-LC High Resolution SWATH-MS of Vaccine Samples under Development**; Søren Heissel¹; Milla Neffling²; Rikke Raaen Lund³; Thomas Kofoed³; Marie Grimstrup³; Nick Morrice²; Anne Fich Holmbjerg⁴; Max Per Kristiansen⁴; Ingrid Kromann⁴; Peter Højrup¹; Ejvind Mørtz³; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; ²SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; ³Alphalyse A/S, Odense M, DK; ⁴Statens Serum Institut, Copenhagen, Denmark
- WP 629 **Highly Sensitivity and Reproducible MRM Based Quantitation of Follicle Stimulating Hormones (FSH) in Human Plasma using QTRAP™ 6500**; Faraz Rashid¹; Rahul Baghla²; Prashant Kale³; Manoj Shukla³; Milin Shah³; Dipankar Malakar²; Anoop Kumar²; Manoj Pillai²; ¹SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India; ²Sciex Gurgaon, Gurgaon, India; ³Lambda Therapeutic Research Ltd, Ahmedabad, India

- WP 630 **Streamlining the Complete Sequence Variant Analysis Workflow for Biotherapeutics**; Andrew Dawdy¹; Michelle English²; Mellisa Ly²; Andrew Saati²; Lisa A Marzilli²; Olga Friese¹; Jason C Rouse²; Yong J Kil³; Marshall Bern³; Eric Carlson³; Chris Becker³; ¹Pfizer, Inc. Chesterfield, MO; ²Pfizer, Inc. Andover, MA; ³Protein Metrics Inc., San Carlos, CA
- WP 631 **Comparison of First Dimension Fractionation Strategies for Directed MS Analysis of Host Cell Proteins**; Jordy Hsiao¹; Te-Wei Chu¹; Gregory O Staples¹; Oscar Potter¹; Hongfeng Yin¹; Kevin Killeen¹; ¹Agilent Technologies, Santa Clara, CA
- WP 632 **Determination of Total Recombinant Human α -Galactosidase A in Plasma Samples by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; Rick Hamler¹; Kees Bronsema²; Peter Pruim²; Peter Bults²; Deborah Hilliard¹; Russell Gotschall¹; Franklin K Johnson¹; Hung Do¹; Kenneth Valenzano¹; Nico van de Merbel²; Elfrida R Benjamin¹; ¹Amicus Therapeutics, Cranbury, NJ; ²PRA Health Sciences, Assen, The Netherlands
- WP 633 **Herceptin Quantitation Using Universal and Signature Peptides by Hybrid LBA/LC-MS Method**; XI QIU¹; Daniell Rowles¹; Susan Zondlo¹; John Kolman¹; Zamas Lam¹; ¹QPS, Newark, DE
- WP 634 **Quantitative Analysis of Adalimumab using nano-Surface and Molecular-Orientation Limited (nSMOL) proteolysis and LC/MS/MS**; Deepti Bhandarkar¹; Ravi Krovidi²; Rashi Kochhar¹; Shailendra Rane¹; Shailesh Damale¹; Purushottam Sutar¹; Anant Lohar¹; Ashutosh Shelar¹; Jitendra Kelkar¹; Ajit Datar¹; Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ²Lambda Therapeutic Research, Ahmedabad, India
- WP 635 **SSPAQ: A Subtractive Method for the Parallel Quantification of the Degree of Modification at Every Possible Site of a Protein**; Guillaume Gabant¹; Alain Boyer¹; Martine Cadene¹; ¹CBM CNRS UPR4301, Orleans, France
- WP 636 **Quantification of the Antibody Drug Conjugate, Trastuzumab Emtansine and the Monoclonal Antibody, Trastuzumab in Plasma Using a Generic Kit-Based Approach**; Hua Yang¹; Mary E Lame¹; Erin E Chambers¹; Sherri Naughton¹; ¹Waters Technologies Corporation, Milford, MA
- WP 637 **Applying a Standardized, Kit-based Approach to Achieve 10 ng/mL Infliximab from 35 μ L Plasma**; Mary E Lame¹; Hua Yang¹; Erin E Chambers¹; Sherri Naughton¹; ¹Waters, Milford, MA
- WP 638 **Quantification of Host Cell Proteins in Biotherapeutics using Stable Isotope Labeled Chinese Hamster Ovary Proteins (SIL-CHOP) as an Internal Standard**; Pegah R Jalili¹; Zhiyun Cao¹; Kevin Ray¹; Rong-Rong Zhu²; ¹MilliporeSigma, Saint Louis, MO; ²MilliporeSigma, Bedford, MA
- WP 639 **Host Cell Protein Analysis of Biopharmaceuticals using Automatic Offline Fractionation and LC/MS**; Alex Zhu¹; Jing Chen²; Steve Murphy²; Jordy Hsiao³; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Inc. Madison, WI; ³Agilent Technologies, Santa Clara, CA
- WP 640 **Exploiting His-tags in Recombinant Protein Therapeutics to Introduce Metal Tracers for Tracking Biodistribution of Biopharmaceuticals *in vivo***; Chengfeng Ren¹; Grégoire Bonvin¹; Cedric Bobst¹; Igor A Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, Massachusetts
- WP 641 **Analysis of N-Glycans Released from Monoclonal Antibodies using an ESI-MS-friendly Fluorescent Tag**; Oscar Potter¹; Gregory O Staples¹; Hongfeng Yin¹; Kevin Killeen¹; ¹Agilent Technologies, Santa Clara, CA
- WP 642 **Evaluation of Transferrin Metal Tracers using Native ESI-MS and *in-vitro* Model for Tracking Its Biodistribution with ICP-MS**; Grégoire Bonvin¹; Cedric Bobst²; Igor A Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, Massachusetts; ²University of Massachusetts-Amherst, Amherst, Massachusetts
- WP 643 **Comprehensive HCP Profiling by Targeted and Untargeted Analysis of DIA Mass Spectrometry Data with PRM qualification**; Simion Kreimer¹; Yuanwei Gao¹; Mi Jin²; Nesredin Mussa²; Alexander R. Ivanov¹; Barry L. Karger¹; ¹Barnett Institute and Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; ²Bristol-Myers Squibb, Devens, MA
- WP 644 **A Promising Alternative to SRM-Very-high-resolution selected-ion- Monitoring (vHR-SIM@500k) Enables Ultra-sensitive and Selective Biotherapeutics Quantification**; Yang Qu¹; Bo An¹; Ming Zhang¹; Xiaomeng Shen¹; Shichen Shen¹; Jun Li¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- WP 645 **Significant Throughput Increase in Peptide Mapping/MAM Analysis Using 2D-UPLC**; Cong Wu¹; Hai Yue¹; Sabrina Benchaar¹; ¹Amgen, Inc., Thousand Oaks, CA
- WP 646 **Sulfur-based Characterization of Protein Standards using Isotope Dilution Inductively Coupled Plasma Mass Spectrometry**; Hyun-Seok Lee^{1,2}; Sook Heun Kim¹; Ji-Seon Jeong^{1,3}; Yong-Moon Lee²; Yong-Hyeon Yim^{1,3}; ¹KRISS, Daejeon, Republic of Korea; ²College of Pharmacy, Chungbuk National University, Cheongju, Korea; ³Department of Analytical Sciences for Biology, University of Science and Technology (UST), Daejeon, Korea
- WP 647 **Bioanalysis of Radiolabeled Payload by Isotopic Pattern Deconvolution and LC-MS/MS to Investigate Tissue Distribution of Protein Drug Conjugates**; Wei Qi Chen¹; Wenying Li¹; Jinping Gan¹; ¹Bristol-Myers Squibb Co., Princeton, NJ
- WP 648 **Site-Specific Glycosylation Quantitation of Bioengineered Recombinant Therapeutic Glycoproteins**; Muchena J. Kailemia¹; Wanghui Wei¹; Kalimuthu Karuppanan¹; Jasmine M. Corbin¹; Yanhong Li¹; L My Phu¹; Abhaya Dandekar¹; Xi Chen¹; Somen Nandi¹; Karen McDonald¹; Carlito Lebrilla¹; ¹University of California, Davis, Davis, CA
- WP 649 **Large-scale and Ultra-Sensitive Investigation of Biotherapeutics by A Novel Antibody-Free, Dual-Mechanism Enrichment Strategy**; Ming Zhang¹; Bo An¹; Yang Qu¹; Shichen Shen¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- WP 650 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic**; Wei Fu¹; Bo An¹; Ming Zhang¹; Yang Qu¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY

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- WP 652 **Comprehensive Draft of the HeLa Proteome to a Depth of More than 13,000 Proteins;** Christian Dahl Kelstrup¹; Dorte B Bekker-Jensen¹; Tanveer S Bath¹; Sara C Larsen¹; Michael L Nielsen¹; Jesper V Olsen¹; ¹CPR, University of Copenhagen, Copenhagen, Denmark
- WP 653 **Subtilisin for Large Scale (phospho)proteomics – the Beginning of a Wonderful Love Story?;** Humberto Gonczarowska-Jorge^{1,2}; Stefan Loroch¹; Margherita Dell'Aica¹; René Zahedi³; ¹ISAS, Dortmund, Germany; ²CAPES Foundation, Ministry of Education of Brazil Brasília-Brazil; ³ISAS, Dortmund
- WP 654 **A New Approach to the Analysis of Intact Major Urinary Proteins (MUPs) from Mouse Urine by CESI-MS;** Stephen J. Lock¹; Robert J. Beynon²; Guadalupe Gomez-Baena²; Edna Betgovarguez³; ¹SCIEX, Warrington, Cheshire; ²Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK; ³SCIEX, Concord ON, Canada
- WP 655 **Proteogenomics of HEK293 Cell Line: Identification of Variant Peptides using Deep Proteome Data from the Inter-Laboratory Studies;** Anna Lobas^{1,2}; Dmitry Karpov^{3,4}; Arthur Kopylov³; Elizaveta Solovyeva^{1,2}; Mark Ivanov^{1,2}; Irina Ilina³; Vassily Lazarev⁵; Ksenia Kuznetsova³; Ekaterina Ilgisonis³; Victor Zgoda³; Mikhail V Gorshkov^{1,2}; Sergei Moshkovskii³; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; ²Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; ³Institute of Biomedical Chemistry, Moscow, Russia; ⁴Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, Russia; ⁵Research Institute of Physico-Chemical Medicine, Federal Medico-Biological Agency, Moscow, Russia
- WP 656 **Novel Approaches in de novo Peptide Sequencing and Proteogenomics as Tools to Explore Uncharted Organisms;** Bernhard Blank-Landeshammer¹; Karsten Biß¹; Laxmikanth Kollipara¹; Vera Rieder²; Marleen Stühr³; Tilman Schell⁴; René P Zahedi¹; Markus Pfenninger¹; Jörg Rahnenführer²; Hildegard Westphal³; Albert Sickmann¹; ¹Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; ²Fakultät Statistik, Technische Universität Dortmund, Dortmund, Germany; ³Leibniz Center for Tropical Marine Ecology (ZMT), Bremen, Germany; ⁴Biodiversity and Climate Research Centre (BIK-F), Frankfurt Am Main, Germany
- WP 657 **Proteomic Study of Rhizopus Microsporus Fungus Growing in Presence of Copper;** Meriellen Dias¹; Lidiane Maria de Andrade¹; Enrique Eduardo Rozas¹; Mariana de Paula Eduardo¹; Maria Anita Mendes¹; ¹University of São Paulo, São Paulo, SP
- WP 658 **Identification of Methylation and Phosphorylation in Arginine/Serine-Rich Domains by Electron Transfer Dissociation Mass Spectrometry;** Isaac Bishof¹; Duc M. Duong²; Eric B. Dammer²; Nicholas T. Seyfried²; ¹Emory University, Atlanta, GA; ²Emory University School of Medicine, Atlanta, GA
- WP 659 **Capturing Protein Binders to Yeast Ribosome Biogenesis and Stress Response Genes Using Multiplexed HyCCAPP;** Yunxiang Dai¹; Julia Kennedy-Darling¹; Mark Scalfi¹; Audrey Gasch¹; Lloyd M Smith¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 660 **Elucidation of Dynamic Cell Surface Protein-Protein Interactions using Chemoproteomic Technologies;** Damaris Bausch-Fluck¹; Maria P Pavlou¹; Bernd Wollscheid¹; ¹Institute of Molecular Systems Biology, Dep. of Health Sciences and Technology, ETH Zürich, Zürich, Switzerland
- WP 661 **Development of an On-Slide-Digestion, MS Assay from Formalin-Fixed Paraffin Embedded (FFPE) Breast Tissue;** Ten-Yang Yen¹; Moe Thein²; Roger Yen²; Leslie Timpe²; Bruce Macher²; ¹San Francisco State University, San Francisco, CA; ²San Francisco State University, San Francisco, CA
- WP 662 **Multi-omics Analysis for the Global Proteins and Metabolites in Experimental Autoimmune Myocarditis Rat Model;** Jin Woo Jung¹; Jae Hun Jung²; Kwang Pyo Kim²; Geum-Sook Hwang³; Jungju Seo¹; ¹Korea Basic Science Institute, Daejeon, Republic of Korea; ²Kyung Hee University, Yongin, Republic of Korea; ³Korea Basic Science Institute, Seoul, Republic of Korea
- WP 663 **Multiplexing Targeted Proteomics: Increased Throughput of Targeted Biomarker Measurements using Isobaric Labels and Dedicated MS3 Analysis;** Robert Everley¹; Brian K. Erickson¹; Christopher M. Rose¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA
- WP 664 **Comparative Study on Chemical Derivatization of Lysines to mimic Arg-C digestion;** Vahid Golghalyani¹; Michael Karas¹; ¹Goethe University, Frankfurt Am Main, Germany
- WP 665 **Developing an LC/MS/MS Method for the Identification of Key Secretome Proteins from Human Lung Spheroid Cells;** Dipti Paudel¹; Phuong-Uyen Dinh²; Jhon Cores³; Robert Kevin Blackburn³; Ke Cheng³; Michael Goshe³; ¹NCSU, Raleigh, NC; ²North Carolina State University, Raleigh, NC; ³North Carolina State University, Raleigh, NC
- WP 666 **Evaluation and Establishment of the Method for the Accurate Protein Quantification in the Subcellular Fraction;** Atsushi Sakamoto¹; Akiko Matsui¹; Asami Saito¹; Gaku Morinaga¹; Akiko Takamoto¹; Naoki Ishiguro¹; Shinobu Suzuki¹; ¹Nippon Boehringer Ingelheim, KOBE, JPN
- WP 667 **Fluorescence Complementation Mass Spectrometry (FCMS) for Identifying Direct Upstream Kinases;** Lingfei Zeng; Department of MCMP, Purdue, West Lafayette, IN
- WP 668 **Protein Analysis Using a Combination of an Online Trypsin Immobilized Enzyme Reactor and CAD/ETD Tandem Mass Spectrometry;** Kun Cho¹; Sang Eun Hong²; Kyung Ju Jang²; Kuk Ro Yoon²; Jong Shin Yoo¹; ¹KBSI, Cheongju-Si, S. Korea; ²Hannam University, Daejeon, Korea
- WP 669 **Parallel SUMO/Ubi Profiling Using an Optimized Peptide IP;** Frederic Lamoliatte¹; Francis McManus¹; Ghizlane Maarifi²; Mounira K. Chelbi-Alix²; Pierre Thibault¹; ¹IRIC-Université de Montréal, Montréal, QC; ²INSERM Unité Mixte de Recherche S 1124, Université Paris Descartes, Paris, France
- WP 670 **Electron-Transfer/Higher-Energy Collision Dissociation (ETHCD) Improves Spectral Quality while Retaining Quantitation Accuracy in Isobaric Tag-based Quantitative Proteomic Studies;** Yu Feng¹; Qing Yu¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 671 **A New Digestion Method to Analyze Respiratory Complex I;** Stefan Schoenborn; Department of Pharmaceutical Chemistry, Goethe University, Frankfurt, Germany
- WP 672 **The Establishment of Nano Mass Spectrometry Analysis Techniques for the Identification of Lead Ion Effect in Hemoglobin;** Ming-Hui Yang¹; Yu-Chang Tyan²; ¹Graduate Institute of Medicine, KMU, Kaohsiung, Taiwan; ²Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 673 **A Quantitative Tunable Digestion Approach Uncovers Novel Acetyl and Methyl Marks on Histones;** Chris Adams¹; Nora Yucel²; Allis C Chien²; Ryan D Leib²; ¹Stanford University, Stanford, CA; ²Stanford University, Stanford, CA
- WP 674 **Identification of GHB-binding Proteins by Mass Spectrometry – (Chemo)proteomic Analysis of Synaptosomal Membrane Proteins;** Ulrike Leurs; University of Copenhagen, Copenhagen, Sjaelland

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- WP 675 **Development of Dimethyl Pyrimidinyl Ornithines (DiPyrO) as Mass Defect-Based Tags for Quantitative Proteomics;** Amanda Rae Buchberger¹; Dustin Frost¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 676 **Examining pH Specificity of Peptide N-terminal Amine Tagging Reagents for cPILOT Analysis;** Lindsay Osentoski¹; Yaphet Geadion¹; Joseph Dudenhoeffer¹; Christina King¹; Renā A.S. Robinson¹; ¹University of Pittsburgh, Pittsburgh, PA
- WP 677 **Application of SuperQuant to Obtain Quantitative Information of the Glioblastoma Proteome;** Thiago Verano-Braga¹; Vladimir Gorshkov¹; Sune Munthe²; Mia Dahl Soerensen²; Bjarne Winther Kristensen²; Frank Kjeldsen³; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; ²Odense University Hospital, Odense, DK; ³BMB, Odense M
- WP 678 **Combining of iTRAQ Labeled Peptides from HPLC Fractions: Where is the Limit for Peptides/Proteins Detected and Quantified?;** Trong Khoa Pham¹; Kirsty Richards²; Jo Roobol²; Colin Robinson²; Phillip C. Wright³; ¹Department of Chemical and Biological Engineering, The University of Sheffield, Sheffield, UK; ²School of Biosciences, University of Kent, Canterbury, UK; ³Faculty of Science, Agriculture and Engineering, Newcastle University, Newcastle upon Tyne, UK
- WP 679 **Increasing Protein Quantification in 6-plex TMT Experiments;** Jane Liu¹; Michael Sweredoski²; Sonja Hess²; ¹Pomona College, Claremont, CA; ²California Institute of Technology, Pasadena, CA
- WP 680 **Evaluation of a Pulsed SILAC-TMT Multiplexing Strategy for Measurement of Proteome Dynamics;** Jana Zechar¹; Chen Meng¹; Mathias Wilhelm¹; Susan Klaeger¹; Bernhard Kuster^{1,2}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany
- WP 681 **Extended Mass Range QQQ for Routine Analysis of Large, Low-Charge State Peptide Ions;** Linfeng Wu¹; Christine A Miller¹; ¹Agilent Technologies, Santa Clara, CA
- WP 682 **Pseudo-isobaric Fragment Ions Provide Accurate and Precise Proteome Quantification Results;** Yuan Zhou¹; Jianhui Liu¹; Zhigang Sui¹; Lihua Zhang¹; Yukui Zhang¹; ¹Key Laboratory of Separation Science for Analytical Chemistry; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
- WP 683 **Investigation of Q-TOF Instruments Advantages for label-free Proteome Analysis;** Stephanie Kaspar-Schoenefeld¹; Markus Lubeck¹; Annette Michalski¹; Pierre-Olivier Schmitz¹; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker Daltonique S.A., Wissembourg, France
- WP 684 **Stable-isotope Maleic Anhydride Labeling-based Approach for Quantitative Proteomics;** Kai Zhang¹; Shuzhen Zheng²; Shanshan Tian³; Zhenchang Guo³; Guijin Zhai³; ¹Tianjin Medical University, Tianjin, Tianjin; ²Nankai university, Tianjin, China; ³Tianjin Medical University, Tianjin, China
- WP 685 **Intact Protein Quantitation up to a 1000-fold Using Protein Universal Pseudo-isobaric Dimethylation;** Zhixin Tian¹; Houqin Fang¹; Kaijie Xiao¹; ¹Department of Chemistry, Tongji University, Shanghai, Shanghai
- WP 686 **Evaluation of a Novel Tandem Quadrupole Mass Spectrometer for the Quantitative Analysis of Peptides using a Multi-Point Internal Calibration Method;** Billy Molloy¹; Donald J.L. Jones^{2,3}; Donald P Cooper⁴; Johannes PC Visser⁴; James I Langridge⁴; ¹Waters, Wilmslow; ²Department of Cancer Studies, University of Leicester, UK, Leicester, UK; ³Cardiovascular Research Centre, Glenfield Hospital, Leicester, UK, Leicester, UK; ⁴Waters, Wilmslow, UK
- WP 687 **Comparison of Label-Free and TMT Quantification for Global Phosphoproteome Analysis of Apoptotic Cells;** Emmanuelle Lezan¹; Christoph Schmutz¹; Simon Josef Ittig¹; Erik Ahnér¹; Alexander Schmidt¹; ¹Biozentrum, University of Basel, Basel, Switzerland
- WP 688 **Examining Proton Transfer and Ion Scattering for Intact Proteins in a Triple Quadrupole Mass Spectrometer;** Evelyn H Wang¹; Dananjaya Kalu Appulage¹; Erin A. McAllister²; Kevin A Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²Shimadzu Scientific Instruments, Columbia, MD
- WP 689 **α - and β -tubulin Isotype Repertoire Quantification by LC-SRM in Blood Platelet and HeLa Cells;** Agnes Hovasse¹; Magda Magiera²; Catherine Strassel³; Alain Van Dorsselaer⁴; Carsten Janke²; Francois Lanza³; Christine Schaeffer-Reiss⁴; ¹Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, Alsace; ²Institut Curie, Orsay, France; ³UMR_S 949 Inserm, EFS-Alsace, Université de Strasbourg, Strasbourg, France; ⁴Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, France
- WP 690 **Combination of Ultrasensitive Sample Preparation and NHS-chemistry Enables Sensitive Quantification of Lysine Acetylation and Large Proteome Coverage;** Christian Frese¹; Özge Karayel¹; Jeroen Krijgsvel¹; ¹DKFZ German Cancer Research Center, Heidelberg, Germany
- WP 691 **Combining Ion Mobility Enhanced DDA and DIA Workflows for Label-Free Quantitative Phosphoproteomics;** Ute Distler^{1,2}; Pedro Navarro¹; Jennifer Hahlbrock¹; Kuharev Jörg¹; Stefan Tenzer¹; ¹Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany; ²Focus Program Translational Neuroscience (FTN), University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany
- WP 692 **Comprehensive Relative Quantification of the Cytochromes P450 by micro-LC and SWATH® Acquisition and Data Processing using Cloud Computing;** Rosalind E. Jenkins¹; Sibylle Heidelberger²; Thomas Knapman²; Francesco Brancia²; Neil Kitteringham¹; Kevin B Park¹; Mark Carfazzo³; ¹MRC Centre for Drug Safety Science, Liverpool, UK; ²SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; ³Sciex, Redwood Shores, CA
- WP 693 **Interference-free Multiplexed Quantification with Complement Reporter Ions: Technological Advances and Application to Nucleocytoplasmic Partitioning;** Martin Wuehr^{1,2}; Graeme C McAlister³; Thomas Güttler²; Brian K. Erickson²; Matthew Sonnett²; Ramin R. Rad²; Keisuke Ishihara²; Leonid Peshkin²; Aaron C. Groen²; Marc Presler²; Elizabeth Van Itallie²; Wilhelm Haas⁴; Timothy J. Mitchison²; Steven P. Gygi²; Marc W. Kirschner²; ¹Princeton University, Princeton, NJ; ²Harvard Medical School, Boston, MA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Massachusetts General Hospital, Boston, MA
- WP 694 **Veracity or Serendipity? Contradicting Conjectures in Protein Quantification;** Russell P Grant¹; Christopher M Shuford¹; Patricia L Holland¹; ¹Laboratory Corporation of America, Burlington, NC
- WP 695 **A New and Easy Approach for End-User Driven Quantification of SIL Peptide Solutions in Targeted Proteomics;** Karsten Schnatbaum¹; Lars Hornberger¹; Johannes Zerweck¹; Tobias Knaute¹; Lawrence Eckler¹; Ulf

- Reimer¹; Holger Wenschuh¹; ¹JPT Peptide Technologies GmbH, Berlin, Germany; ²JPT Peptide Technologies, Berlin, Germany
- WP 696 **PRM Method Optimization on a Q-Exactive Plus Using a Well-Defined Quantitative Proteomics Standard**; Zhiyun Cao¹; James J Walters²; Kevin B Ray²; ¹MilliporeSigma, St. Louis, Missouri; ²MilliporeSigma, St. Louis, MO
- WP 697 **Optimizing Experimental Design for Ultra-deep Discovery Proteomics of Breast Cancer Patient Derived Xenografts with Isobaric Peptide Labeling**; Qiang Zhang¹; Robert Sprung¹; Petra Erdmann-Gilmore¹; Yiling Mi¹; Rose Connors¹; Sherri Davies¹; Shunqiang Li¹; Reid Townsend¹; ¹Washington University School of Medicine, Saint Louis, MO
- WP 698 **Development of Robust, Reproducible, High-Throughput Quantitative Proteomic Assays for Cellulosic Biofuel Applications**; Yan Chen¹; Leanne Jade G Chan¹; Héctor García Martín¹; Paul D Adams¹; Christopher J Petzold¹; ¹Lawrence Berkeley National Laboratory, Berkeley, CA
- WP 699 **Highly Multiplexed MRM-based Peptide Quantitation in Human Plasma Using Two Different Stable Isotope Labeled Peptides for Calibration**; André LeBlanc¹; Sarah Michaud²; Andrew Percy¹; Darryl B Hardie¹; Juncong Yang¹; Nicholas Sinclair¹; Jillaine Proudfoot¹; Adam Pistawka¹; Derek S Smith¹; Christoph H. Borchers^{3,4}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²MRM Proteomics, Inc., Victoria, BC, Canada; ³University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ⁴Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- WP 700 **Second Generation Combinatorial Mass Tag (CMT) Isobaric Reagents with Improved Quantitative Precision**; Craig Braun¹; Brian Erickson¹; Gregory Bird²; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA; ²Dana Farber Cancer Institute, Boston, MA
- WP 701 **Utilizing Synthetic Peptides and Skyline for Validating Quantitative Changes in Bacterial Proteomics**; Chia-Fang Lee¹; Chen-Hsun Tsai¹; Lydia M. Contreras¹; Maria D. Person¹; ¹University of Texas at Austin, Austin, TX
- WP 702 **A Peptide-Retrieval Strategy Enables Significant Improvement of Quantitative Performance Without Compromising Confidence of Identification**; Chengjian Tu¹; Shichen Shen¹; Quanhu Sheng²; Yu Shyr²; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Vanderbilt University, Nashville, TN
- WP 703 **Multiplexing Quantification of Proteins by Single-Cell CE- μ ESI-HRMS Finds Translational Cell Heterogeneity in the 16-cell Frog (Xenopus) Embryo**; Camille Lombard-Banek¹; Sally A Moody¹; Peter Nemes¹; Sushma Reddy¹; ¹The George Washington University, Washington, DC
- WP 704 **Secretome Profiling of Antibody-Producing CHO Cells using Non-Natural Amino Acid Crosslinking Pull Down and Mass Spectrometry**; Carlo Martins¹; Raghothama Chaerkady¹; Michael Bowen¹; Deniz Baycin-Hizal¹; ¹MedImmune, Gaithersburg, MD
- WP 707 **Development and Validation of an Ultra Sensitive and Automated LC-MS/MS Method for the Measurement of Naloxone, Buprenorphine and Norbuprenorphine**; Nick Peng¹; Ben Gaboury¹; Nichole Boice¹; Dan Pederson¹; Ardeshir ardeshir khakang¹; ¹Axis Clinicals, Dilworth, MN
- WP 708 **Development and Validation of a Simple, Rugged and Automated LC-MS/MS Method for the Determination of Mesalamine in Human Plasma**; Nick Peng¹; BEN GABOURY¹; Sarah Maasjo¹; Ardeshir Khadang¹; ¹Axis Clinicals, Dilworth, MN
- WP 709 **Simultaneous Determination of Tamsulosin and Solifenacin in Human Plasma by Ultra-High Performance Liquid Chromatography with Tandem Mass Spectrometry**; Jin Sun Woo¹; Hwa Suk Kim¹; Seo Hyun Yoon¹; Joo-Youn Cho¹; ¹Seoul National University College of Medicine, Seoul, South Korea
- WP 710 **Applications of Improved GCMS Method for Fatty Acid Analysis in Samples from Bariatric Patients and Mice Fed Omega-3 Fatty Acids**; Kazimierz Surowiec¹; Nadeeja N. Wijayatunga¹; Latha Ramalingam¹; Valerie G. Sams²; Gregory J. Mancini²; Matthew L. Mancini²; Yehia Mechref¹; Naima Moustaid-Moussa¹; ¹Texas Tech University, Lubbock, TX; ²University of Tennessee Medical Center, Knoxville, TN
- WP 711 **A Two-dimensional Liquid Chromatography (2D-LC) to Separate an Interference Peak from Norfentanyl for Its Successful Bioanalysis**; Moo-Young Kim¹; Brendan Laing¹; Fumin Li¹; ¹PPD, Middleton, WI
- WP 712 **Development and Validation of a LC-MS/MS Method for the Simultaneous Quantitation of Carboplatin and Etoposide in Human Plasma and Ultrafiltrate**; Jessica Sima¹; Ganesh S Moorthy²; Athena Zuppa²; Elizabeth Fox²; ¹Children's Hospital of Philadelphia, Philadelphia, PA; ²Children's Hospital of Philadelphia, Philadelphia, PA
- WP 713 **Highly Accurate Sample Collection, Handling and LCMSMS Bioanalysis of Liposomal Amphotericin B Plasma Samples**; Jason Bilodeau¹; François Viel¹; Nadine Boudreau¹; Clark Williard¹; ¹inVentiv Health, Québec, Canada
- WP 714 **Determination of Unconjugated Naloxone, Conjugated Naloxone and Total Naloxone in Human Plasma by LCMSMS**; Louis-Charles Boisvert¹; Nicolas Jean¹; Guy Havar¹; Philippe Belanger¹; Marie-Josée Marcoux¹; Sylvain Lachance¹; Nadine Boudreau¹; Clark Williard¹; ¹inVentiv Health, Québec, Canada
- WP 715 **Trace Level Quantitative Determination of Phthalates from High Risk Dosage Pharmaceutical Formulations using LC/MS/MS**; Purushottam Sutar¹; Rashi Kochhar¹; Deepti Bhandarkar¹; Shailendra Rane¹; Shailesh Damale¹; Anant Lohar¹; Ashutosh Shelar¹; Jitendra Kelkar¹; Pratap Rasam¹; Ajit Datar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- WP 716 **Highly Sensitive Multiplexed Analysis of Levosalbutamol from Plasma using LC/MS/MS**; Ashutosh Shelar¹; Shailesh Damale¹; Shailendra Rane¹; Purushottam Sutar¹; Anant Lohar¹; Deepti Bhandarkar¹; Rashi Kochhar¹; Pratap Rasam¹; Jitendra Kelkar¹; Ajit Datar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- WP 717 **Robust, Sensitive and Accurate Determination of Different Opioids in Human Plasma by LCMSMS**; Genevieve Emond¹; Marc Fournier¹; Marie-Claude Thérberge¹; Nathalie Pelletier¹; Marie-Josée Marcoux¹; Sylvain Lachance¹; Nadine Boudreau¹; Clark Williard¹; ¹inVentiv Health, Québec, Canada
- WP 718 **Simultaneous Assay of Multiple Synthetic Contraceptive Hormones in Human Serum by LCMS-MS**; Steven W Blue¹; Rachel Lieberman²; David W Erikson¹; Christopher Gilles²; ¹Oregon National Primate Research Center, Beaverton, OR; ²Shimadzu Scientific Instruments, Columbia, MD

SMALL MOLECULES: QUANTITATIVE ANALYSIS (PART 1) 705 - 728

- WP 705 **Dilute and Shoot FI-MS/MS for Quantification of Glycocholic Acid in Human Bile using Standard Addition Method**; Raghavi Kakarla¹; Ramakrishna reddy Voggu¹; Janet R Donaldson²; Baochuan Guo¹; ¹Cleveland State University, Cleveland, OH; ²Mississippi State University, Starkville, MS
- WP 706 **Development of Cost-Effective Liquid Chromatography-Tandem Mass Spectrometry Method for Polar Drugs and Metabolites**; Xiaodong Zhu¹; Jingguo Hou¹; Jerry Gardella¹; Melvin Tan¹; Tom Lloyd¹; Edward Wells¹; ¹Worldwide Clinical Trials Drug Development Solution, Austin, TX



- WP 719 **Highly Sensitive Automated Assay for the Determination of Oxytocin in Human Plasma by LC-MS/MS;** Nicolas Jean¹; Philippe Bélanger¹; Carine Lévesque¹; Marie-Claude Théberge¹; Nadine Boudreau¹; Clark Williard¹; Hermes Licea-Perez²; Jonathan Kehler²; Thomas Mencken²; ¹*inVentiv Health, Québec, Canada*; ²*GlaxoSmithKline, Upper Merion, PA*
- WP 720 **Quantification of Tenofovir and Emtricitabine in Human Plasma using High Throughput LDTD-MS/MS;** Jean Lacoursiere¹; Annie-Claude Bolduc²; Alex Birsan¹; Serge Auger¹; Pierre Picard¹; ¹*Phytronix Technologies, Inc. Québec, Canada*; ²*Université Laval, Québec, Canada*
- WP 721 **A Sensitive LC-MS/MS Method for Quantitation of Naltrexone and 6 β -Naltrexol in Human Plasma (1 pg/mL);** Dawei Zhou¹; Shaoting Zhang¹; Mohamed Osman¹; Xinping Fang¹; ¹*WuXi AppTec Co., Plainsboro, NJ*
- WP 722 **Quantification of N-Hydroxy Riluzole Metabolite in Human Plasma: The Investigation of the Stability of the Analyte;** Luc Bouchard¹; Nathalie Pelletier¹; Sylvain Lachance¹; Nadine Boudreau¹; Clark Williard¹; ¹*inVentiv Health, Québec, Canada*
- WP 723 **Ultra-Sensitive LCMSMS Determination of Teriparatide in Human Plasma;** Philippe Bélanger¹; Marie-Josée Marcoux¹; Nadine Boudreau¹; Clark Williard¹; ¹*inVentiv Health, Québec, Canada*
- WP 724 **Development of an Ultrasensitive Assay for Quantification of Free Ticagrelor in Plasma using Equilibrium Dialysis and LC-MS/MS;** Ann-Sofie Sandinge¹; Annika Janefeldt¹; ¹*AstraZeneca R&D, Gothenburg, Sweden*
- WP 725 **Bioanalytical LC/MS/MS Method for the Determination of a Vitamin E analog in Human Plasma;** Jeff Jeppson¹; Elizabeth Dibbern¹; Ridha Nachi¹; ¹*Celerion, Lincoln, NE*
- WP 726 **Comparison of the Quantitation of Bile Acids using Full Scan and Targeted SIM Mode on using UPLC/HRAM MS;** Brandon Wilcock¹; Lijuan Fu¹; Nan Zhao¹; Cassidy Hatch¹; Nidhi Jaiswal¹; Min Meng¹; Troy Voelker¹; Scott Reuschel¹; ¹*Covance, Salt Lake City, UT*
- WP 727 **A Selective and Ultra-Sensitive LC-MS/MS Method for Simultaneous Quantitation of Norgestrel and Norgestimate in Human Plasma;** Shuyu Hou¹; Sheth Raj¹; Hongkun Liang¹; Yuan-Shek Chen¹; Hsu Ben¹; ¹*QPS, LLC, Newark, DE*
- WP 728 **Rapid Analysis of Ceftriaxone in Human Intestinal Chyme, Human Plasma, and Dog Plasma by HPLC/MS/MS;** Todd Lusk¹; John F Kokai-Kun²; Michael Schlosser³; Stacey Zeman¹; Sara Brady¹; Daniel 1 Mulvana⁴; Thad Yousey⁵; ¹*Q² Solutions Bioanalytical and ADME Labs, Ithaca, NY*; ²*Synthetic Biologics, Inc., Rockville, MD*; ³*MSR Pharma Services, Inc., Lincolnshire, IL*; ⁴*Q² Lab Solutions Bioanalytical and ADME Labs, Ithaca, NY*; ⁵*Quintiles, Ithaca, NY*

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

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Biomarkers: Quantitative Analysis (Small Molecules & Metabolites).....		059 - 089
Drug Metabolism: Quantitative Analysis.....		090 - 107
Food Safety: Other Contaminants (Part 2).....		108 - 141
GCMS: Instrumentation and Applications (Applications).....		142 - 171
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Proteomics: Quantitative (Pre-MS and Platforms/Informatics/ MultiOmics/Dynamics).....		626 - 649
Proteomics: Tissue.....		650 - 675
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Systems Biology (Protein Modifications and Cells).....		699 - 719
Toxicology.....		720 - 748

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION (DART/PLASMA, LASER, SAWN) 001 - 030

- ThP 001 **Dopant-Assisted Direct Analysis in Real Time (DART) Ionization with Argon Gas;** Robert B. Cody¹; A. John Dane¹; ¹JEOL USA Inc., Peabody, MA
- ThP 002 **Method Development of High Throughput Lipid Analysis in Foods by Direct Analysis in Real Time Mass Spectrometer (DART-MS);** Jun Watanabe¹; Sakakura Motoshi²; Shiota Teruhisa²; ¹Shimadzu Corporation, Kyoto; ²AMR Inc., Tokyo, Japan
- ThP 003 **Acoustically Levitated Drops: A Containerless Microreactor Coupled with Ambient Ionization Mass Spectrometry;** Elizabeth A Crawford¹; Cemal Esen²; Dietrich A Volmer¹; ¹Saarland University, Saarbrücken, Germany; ²Ruhr-University Bochum, Bochum, Germany
- ThP 004 **Application of Direct Analysis in Real Time-Mass Spectrometry to the Study of Oxidation of Skin Oil Components with Indoor Ozone;** Shouming Zhou¹; Matthew Forbes²; Jonathan P D Abbott¹; ¹University of Toronto, Toronto ON, Canada; ²Department of Chemistry, University of Toronto, Toronto, ON
- ThP 005 **Development of a Flavor Release Analysis Method on Volatile Compounds of Citrus Fruits by DART MS;** Sagawa Takehiko¹; Matsumoto Keiko²; Watanabe Jun²; Takei Chikako³; Sakakura Motoshi⁴; Shiota Teruhisa⁴;

Matsufuji Hiroshi⁵; ¹S & B Foods Inc., Tokyo, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Bio Chromato, Inc. Fujisawa, Japan; ⁴AMR Inc., Tokyo, Japan; ⁵Nihon University, Fujisawa, Japan

- ThP 006 **Direct Quantification Technique for Natural Moisturizing Factor (NMF) in Stratum Corneum by Direct Analysis in Real Time Mass Spectrometry (DART-MS);** Katsuyuki Maeno¹; Yasuo Shida²; Haruo Shimada¹; ¹Shiseido Global Innovation Center, Yokohama, Japan; ²University of Yamanashi, Kofu, Japan
- ThP 007 **Accurate Quantification of Urinary Creatinine by Stable Isotope Dilution and DART Coupled to Quadrupole Time-of-Flight Mass Spectrometry;** Ning Zhang^{1,2}; Yuanyuan Song¹; Meiling Lu³; Weibing Zhang²; Hailin Wang¹; Xiaokun Duan⁴; Charles C. Liu⁴; ¹Research Center for Eco-Environmental Sciences, Beijing, China; ²East China University of Science and Technology, Shanghai, China; ³Agilent Technologies (China) Limited, Beijing, China; ⁴ASPEC Technologies LTD, Beijing, China
- ThP 008 **Research of Real-Time Monitoring Method for Volatiles in Chinese Liquor (Baijiu) Tasting;** Ming Liu¹; Zijing Xu²; Jianghao Lu¹; Yi Zhang²; Qiding Zhong¹; Xiaomei Yuan¹; Zhenghe Xiong¹; Xiaokun Duan³; Kai Liu³; ¹China National Research Institute of Food & Fermentation Industries, Beijing, China; ²Sichuan Jiannanchun Group Co. Ltd, Mianzhu, Sichuan; ³ASPEC Technologies LTD, Beijing, China
- ThP 009 **Screening Analysis of Primary Aromatic Amines in Textiles using DART-MS;** Yamamura Yutaro¹; Maeda Kengo²; Jun Watanabe³; Sakakura Motoshi⁴; Shiota Teruhisa⁴; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Co., Kyoto, Japan; ³Shimadzu Corporation, Kyoto; ⁴AMR Inc., Tokyo, Japan
- ThP 010 **A Study of DART® as a Technique for Ambient Surface Analysis of Polymers;** Dana Reed¹; Katri Huikko¹; Steven Pachuta¹; Ali Rafati¹; ¹3M Corporation, St. Paul, MN
- ThP 011 **On-line Coupling of Surface Plasmon Resonance to Ambient Mass Spectrometry;** Huwei Liu¹; Yiding Zhang²; Yu Bai²; ¹Peking University, Beijing; ²Peking University, Beijing, China
- ThP 012 **An Interface for Online Coupling Surface Plasmon Resonance with Mass Spectrometry using Dielectric Barrier Discharge Ionization;** Yiding Zhang¹; Yu Bai¹; Huwei Liu¹; ¹Peking University, Beijing, China
- ThP 013 **Determination of Peroxide Explosives and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS);** Sebastian Hagenhoff¹; Heiko Hayen¹; ¹University of Muenster, Muenster, Deutschland
- ThP 014 **Surface Erosion and Analysis of Polymer Sample via Micro Dielectric Barrier Plasma Jet Mass Spectrometry;** Songyue Shi¹; Xiaoxia Gong¹; Xinyue Liang¹; Gerardo Gamez¹; ¹Texas Tech University, Lubbock, TX
- ThP 015 **Low Temperature Plasma Desorption/Ionization Mass Spectrometry for Quantitative Analysis of Exhaled Breath Collected on Filter Substrates;** Xiaoxia Gong¹; Songyue Shi¹; Xinyue Liang¹; Mohammad Choudhury¹; Gerardo Gamez¹; ¹Texas Tech University, Lubbock, TX
- ThP 016 **Effects of Molecular Gas Addition on a Helium Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Desorption/Ionization (ADI) Source;** Sunil Badal¹; Jacob T. Shelley¹; ¹Department of Chemistry and Biochemistry, Kent State University, Kent, OH
- ThP 017 **Reactive Ambient Mass Spectrometry with Flowing Atmospheric Pressure Afterglow;** Gerardo Gamez¹; Xiaoxia Gong¹; Xinyue Liang¹; Songyue Shi¹; Mohammad Choudhury¹; ¹Texas Tech University, Lubbock, TX
- ThP 018 **A Microwave Plasma for Simultaneous Molecular and Atomic Ambient Ionization of Solids;** Kenyon Evans-

- Nguyen¹; Jon Gerling²; Ashley Windom³; ¹University of Tampa, Tampa, FL; ²Gerling Applied Engineering, Modesto, CA - California; ³The University of Tampa, Tampa, FL
- ThP 019 **Automatic Analyte Ion Recognition and Background Removal for Ambient Mass Spectrometry Data Based on Cross Correlation**; Yi You¹; Sunil P. Badal¹; Jacob T. Shelley¹; ¹Department of Chemistry and Biochemistry, Kent State University, Kent, OH
- ThP 020 **Characterization of Chemical Noise in AP MALDI using LTQ and Orbitrap Mass Spectrometer**; Eugene Moskovets¹; Vladimir M Doroshenko²; Shelley N Jackson³; Amina S Woods³; ¹MassTech Inc, Columbia, MD; ²MassTech, Inc Columbia, MD; ³NIDA-IRP, NIH Baltimore, MD
- ThP 021 **Magnetic-Field-Assisted Laser-Ablation Ambient Mass Spectrometry**; Yao Lu¹; Yun Shen Zhou¹; Lei Liu¹; Xi Huang¹; Yongfeng Lu¹; ¹Department of Electrical and Computer Engineering, University of Nebraska-Lincoln, Lincoln, NE
- ThP 022 **Sensitivity Improvement of Infrared Laser Atmospheric Pressure Ionization Mass Spectrometry by Synchronizing a Q-TOF Mass Spectrometer and the Laser Pulse**; Hashiya Homare¹; Iguchi Yasunari²; Hazama Hisanao²; Awazu Kunio²; ¹Osaka University, Suita; ²Osaka University, Suita, Japan
- ThP 023 **Coaxial Gas Flow Enhances Sample Plume Transfer Efficiency for Remote Laser Ablation Electrospray Ionization Mass Spectrometry**; Jarod Fincher¹; Brent Reschke²; Nicholas Morris²; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²Protea Biosciences, Inc. Morgantown, WV
- ThP 024 **Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Identify Microorganisms at Species Level from Pure and Mixed Cultures**; Simon Cameron¹; Frankie Bolt¹; Adam Burke¹; Zsolt Bodai¹; Alvaro Perdones-Montero¹; Julia Balog²; Tamas Karancsi²; Daniel Simon²; Richard Schaffer²; Tony Rickards³; Kate Hardiman¹; Monica Rebec³; Zoltan Takats¹; ¹Imperial College London, London, UK; ²Waters Research Center, Budapest, Hungary; ³Imperial College Healthcare NHS Trust, London, UK
- ThP 025 **Surface Acoustic Wave Nebulization Sample Introduction for Vacuum-Assisted Plasma Ionization**; Stephen Zambrzycki¹; Matthew C Bernier²; Joel Keeler²; Sung Hwan Yoon³; David R Goodlett³; Facundo M Fernandez²; ¹Georgia Institute of Technology, Atlanta, Georgia; ²Georgia Institute of Technology, Atlanta, GA; ³University of Maryland School of Pharmacy, Baltimore, MD
- ThP 026 **Surface Acoustic Wave Nebulization – Mass Spectrometry: A Tool for Rapid Analysis of Food Products**; Gloria S Yen¹; Thomas Schneider²; Benjamin L Oyler²; Sung Hwan Yoon²; Tao Liang²; David P A Kilgour³; Erik Nilsson¹; David R Goodlett^{1,2}; ¹Deurion LLC, Seattle, WA; ²University of Maryland, School of Pharmacy, Baltimore, MD; ³Nottingham Trent University, School of Science & Technology, Nottingham, UK
- ThP 027 **Performance Characterization of Surface Acoustic Wave Nebulization for Lipid A Mass Spectrometric Analysis**; Tao Liang¹; Thomas Schneider²; Sung Hwan Yoon²; Benjamin L Oyler²; Andrew Dennison³; Gloria S Yen⁴; Yue Huang⁴; Adam A Stokes⁵; Anthony J Walton³; Robert K Ernst⁶; Erik Nilsson⁴; David R Goodlett^{2,4}; ¹University of Maryland School of Pharmacy, Baltimore, MD; ²School of Pharmacy, University of Maryland Baltimore, MD; ³School of Chemistry, The University of Edinburgh, Edinburgh, UK; ⁴Deurion LLC, Seattle, WA; ⁵School of Engineering The University of Edinburgh, Edinburgh, UK; ⁶University of Maryland Baltimore School of Dentistry, Baltimore, MD
- ThP 028 **Surface Acoustic Wave Nebulization – Mass Spectrometry on a TripleTOF Mass Spectrometer**; Thomas Schneider¹; Benjamin L Oyler¹; Larry J Campbell²; Yves J C LeBlanc³; Tom Covey³; Gloria S Yen⁴; Erik Nilsson⁴; David R Goodlett¹; ¹University of Maryland School of Pharmacy, Baltimore, MD; ²AB SCIEX, Concord, Canada; ³AB SCIEX, Concord ON, Canada; ⁴Deurion LLC, Seattle, WA
- ThP 029 **Rapid Identification of Adulterated Edible Oils by DART-QTOF system**; Tanxi Cai¹; Xiaokun Duan²; Peng Wu³; Lili Niu³; Fuquan Yang³; Charles C. Liu²; ¹Institute of Biophysics, CAS, Beijing, China; ²ASPEC Technologies LTD, Beijing, China; ³Institute of Biophysics, CAS Beijing, China
- ThP 030 **Analysis of Metallocene using Atmospheric Pressure Chemical Ionization and Atmospheric Pressure Photo Ionization Coupled with Ion Mobility Mass Spectrometry**; Mathilde Farenc^{1,2,3}; Budagwa Assumani^{1,3}; Carlos Afonso^{2,3}; Pierre Giusti^{1,3}; ¹TOTAL Refining and Chemicals, TRTG Gonfreville l'Orcher, France; ²Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; ³TOTAL RC - CNRS Joint Laboratory C2MC :Complex Matrices Molecular Characterization, France
- BIOMARKERS: DISCOVERY (PART 2)**
031 - 058
- ThP 031 **Non-Target Urinary and Serum Metabonomic Study of Radix Astragali Treated on Rheumatoid Arthritis Rats Using UPLC-Q-TOF-HDMS**; Zhiqiang Liu¹; Tengfei Xu¹; ¹Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, CN
- ThP 032 **Potential Diagnostic Biomarkers and Pathway Analysis of Ovarian Cancer by Lipidomics**; Yangyang Zhang¹; ¹Institute of Chemistry, Chinese Academy of Sciences, Beijing, China
- ThP 033 **Death Domain Associated Protein DAXX May Regulate a Distinct Lipid Metabolism Signature in Breast Cancer**; Iqbal Mahmud¹; Timothy J Garrett¹; Daiqing Liao¹; ¹University of Florida, Gainesville, FL
- ThP 034 **Identification of Unusual Bile Acids as Biomarkers for Niemann-Pick C Disease Using Charge-Remote Fragmentation of N-(4-Aminomethylphenyl)Pyridinium Derivatives**; Xuntian Jiang¹; Laurel Mydock^{1,2}; Fong-Fu Hsu¹; Douglas Covey¹; David E Scherrer¹; Rohini Sidhu¹; Forbes D Porter³; Nicole M Yanjanin³; Dennis J Dietzen¹; Jean Schaffer¹; Daniel Ory¹; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University in St. Louis, St. Louis, MO; ³NIH/NIAID, Bethesda, MD
- ThP 035 **Human Plasma Lipidome Variations in Active Tuberculosis**; Huipeng Neo^{1,2,3}; Shanshan Ji⁴; Federico Torta⁴; Anne K Bendt⁴; Cynthia Chee⁵; Yee Tang Wang⁵; Pavanish Kumar⁶; Bhairav Paleja⁶; Amit Singhal⁶; Gennaro De Libero⁶; Markus R Wenk⁴; ¹NUS Singapore, Singapore, Singapore; ²Agilent Technologies Pte Ltd, Singapore, Singapore; ³Department of Biological Sciences, Singapore, Singapore; ⁴National University of Singapore, Singapore, Singapore; ⁵Tuberculosis Unit, Tan Tock Seng Hospital, Singapore, Singapore; ⁶Singapore Immunology Network (SigN), A*STAR, Singapore, Singapore
- ThP 036 **Mass Spectrometry-Based Metabolomics for Biomarker Discovery after Angioplasty**; Yatao Shi¹; Bowen Wang¹; Xudong Shi¹; Lian-Wang Guo¹; K. Craig Kent¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 037 **Lysophosphatidylinositol: A Novel Biomarker of Ischemia and a Potential Prognostic Indicator of Cardiac Arrest**; Koichiro Shinozaki¹; Tai Yin¹; Junhwan Kim¹; ¹The Feinstein Institute for Medical Research, Manhasset, NY
- ThP 038 **Following Biomarkers of Central Metabolism in Muscles from Diabetic Mouse Model: Metabolic Pathway Imaging**; Juliette Masurel¹; Gregory Hamm¹; Philippe Delataille²; Corinne Foucart²; David Bonnel¹

- Carole Belanger²; Raphael Darteil¹; Jonathan Stauber¹; ¹ImaBiotech, MS Imaging Dept. LOOS, France; ²Genfit, Loos, France
- ThP 039 **Analysis of Volatile Organic Compounds in Pleural Effusions by HS-SPME-cryo-trap-GC/MS**; Zhongping Huang¹; Jie Zhang¹; Huijun Liu¹; Lili Wang¹; ¹Zhejiang University of Technology, Hangzhou, China
- ThP 040 **Controlling the Misuse of Anabolic Steroids by Steroidal Biomarkers Profiling**; Kin-Sing Wong¹; George H.M. Chan¹; Emmie N.M. Ho¹; Terence S.M. Wan¹; ¹Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, China
- ThP 041 **Serum Total Fatty Acids as Potential Biomarkers for Differentiate Benign Lung Diseases from Lung Cancer**; Junling Ren¹; Zhili Li²; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; ²IBMS, CAMS&PUMC, Beijing
- ThP 042 **Modeling the Exposome Paradigm: Exposure Analysis of the Western Honey Bee**; Chloe Wang¹; Malia Wenny¹; Robert L Broadrup¹; Christopher Mayack²; Anthony Macherone^{3,4}; ¹Haverford College, Haverford, PA; ²Swarthmore College, Swarthmore, PA; ³Agilent Technologies, Wilmington, DE; ⁴Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 043 **Proteomics of Human Plasma in Heart Failure with Preserved Ejection Fraction (HFpEF) using Novel Chemical Affinity, Mixed Mode Matrix (M3)**; Richard Mbasu¹; Donald DL Jones²; Liam M Heaney²; Leong L Ng²; Sandhu K Jatinderpal²; Paulene Quinn²; Daniel C Chan²; ¹University of Leicester, Leicester, Leicestershire; ²University of Leicester, Leicester, UK
- ThP 044 **Mass Spectrometry Based Proteomics to Investigate and Characterize the Jumping Translocation Breakpoint (JTB) Protein using Cancer Cell Lines**; Devika Channaveerappa¹; Kangning Li¹; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY
- ThP 045 **Label-free Shotgun Proteomics Identifies Markers of Inflammation from Fetal Fibroblasts**; Owen E Branson¹; Brian C Wulff¹; Miranda L Gardner¹; Traci A Wilgus¹; Michael A. Freitas¹; ¹Ohio State University, Columbus, OH
- ThP 046 **Mass Spectrometry Based Proteomic Investigation of Plasma Samples from Children with Autism Spectrum Disorder (ASD) and Matched Controls**; Kelly Wormwood¹; Megan M Borland¹; Emmalyn J Dupree¹; Alisa G Woods¹; Blythe Corbett²; Costel C Darie¹; ¹Clarkson University, Potsdam, NY; ²Vanderbilt University, Nashville, TN
- ThP 047 **Using LC-MS/MS and Stable Isotope Tracers to Explore Circulating Biomarkers for the Kinetics of Liver Fibrosis**; Haihong Zhou¹; Yangqing Kan²; Ying Chen²; Ye Tian²; Yongcheng Huang²; Yonghua Zhu²; Taro Akiyama²; David Kelley²; Stephen Previs²; Shirley Pinto²; ¹Merck & Co., Inc., Kenilworth, NJ; ²Merck & Co, Kenilworth, NJ
- ThP 048 **Quantitative Proteomic Analysis of Serum Exosomes from Patients with Pancreatic Cancer Reveals the Differentially Expressed Proteins after Chemo-/Radio-Treatment**; Mingrui An¹; Zhijing Tan²; Jianhui Zhu²; Jing Wu²; Jun Cao²; Rui Yang²; Xiucong Pei²; David M. Lubman²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan Medical Center, Ann Arbor, MI
- ThP 049 **Development of an Integrated and Effective Pipeline for Profiling Microbial Proteins from Mouse Fecal Samples by LC-MS/MS**; Jing Wu¹; Jianhui Zhu¹; Haidi Yin¹; Mingrui An¹; Nicholas Pudlo¹; Eric Martens¹; Grace Chen¹; David M Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- ThP 050 **CD90 Expression is Associated with Pancreatic Intraepithelial Neoplasias**; Xiucong Pei¹; Jianhui Zhu¹; Rui Yang¹; Jiaqi Shi²; Zhijing Tan¹; Mingrui An¹; David M Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Michigan Medical School, Ann Arbor, MI
- ThP 051 **Facilitate Biomarker Discovery using Integrated "Omics" Differential Analysis with High Resolution Accurate LC/MS Approach**; Reiko Kiyonami¹; Julian A Saba²; Sergei I Snovidia³; David Peake²; Devin Drew²; Andreas Huhmer²; Ken Miller²; ¹ThermoFisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Rockford, IL
- ThP 052 **Proteomic Analysis of Minute Amount of Colonic Biopsy Samples from Patients by Enteroscopy for Biomarker Discovery**; Xing Liu¹; Zhou Hu¹; Xu Yanli²; ¹Chinese Academy of Sciences, Shanghai, China; ²Fuyang People's Hospital, Fuyang, China
- ThP 053 **Early Diagnostic Biomarkers for Acute Liver Transplantation Rejection**; Su Jung Kim¹; Ji Hyun Kim¹; Na Young Kim¹; Shin Hwang²; Hyun Ju Yoo³; ¹Asan Institute for Life Sci, Asan Medical Center Seoul, South Korea; ²Dep. Liver Transplantation and Hepatobiliary Surgery, Asan Medical Center, Seoul, Republic of Korea; ³Biomedical Research Center, Asan Institute for Life Sciences, Asan Medical Center, Seoul, Seoul
- ThP 054 **The Identification of Biomarkers of Normobaric Hypoxia and Recovery via Exhaled Breath**; Sean Harshman¹; Brian Geier²; Leslie Drummond³; Laura Flory²; Maomian Fan⁴; Jeffrey Phillips³; Darrin Ott⁵; Claude Grigsby⁴; ¹UES Inc, Air Force Research Laboratory, WPAFB, OH; ²UES, WPAFB, OH; ³Naval Medical Research Unit-Dayton, WPAFB, OH; ⁴Air Force Research Laboratory, WPAFB, OH; ⁵US AF School of Aerospace Medicine, WPAFB, OH
- ThP 055 **Integration of Tissue and Urine Proteomes for Biomarker Discovery and Verification of Renal Cell Carcinoma**; Yi-Ting Chen^{1,2,3}; Chien-Lun Chen^{4,5}; Jau-Song Yu^{2,3}; Pei-Chia Wang²; Hsiao-Wei Chen²; Ying-Hsu Chang^{6,7}; Yu-Sun Chang^{2,3}; Ting Chung²; Tsung-Shih Lin²; ¹Department of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; ²Molecular Medicine Research Center, College of Medicine, Chang Gung University, Taoyuan, Taiwan; ³Graduate Institute of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; ⁴Department of Urology, Chang Gung Memorial Hospital, Taoyuan, Taiwan; ⁵School of Medicine, College of Medicine, Chang Gung University, Taoyuan, Taiwan; ⁶Division of Urology, Department of Surgery, LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan; ⁷Graduate Institute of Clinical Medical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan
- ThP 056 **N-terminal Endogeneous Fragments of Tau in Human Cerebrospinal Fluid**; Gunnar Brinkmalm¹; Claudia Cicognola¹; Erik Portelius¹; Henrik Zetterberg^{1,2}; Kaj Blennow¹; Kina Höglund^{1,3}; ¹University of Gothenburg, Mölndal, Sweden; ²UCL Institute of Neurology, London, UK; ³Karolinska Institutet, Huddinge, Sweden
- ThP 057 **Developing a Lysosomal Panel for Biomarker Discovery in Neurodegenerative Diseases using PRM**; Simon Sjödén¹; Gunnar Brinkmalm¹; Annika Öhrfelt¹; Henrik Zetterberg^{1,2}; Kaj Blennow¹; Ann Brinkmalm¹; ¹University of Gothenburg, Mölndal, Sweden; ²UCL Institute of Neurology, London, UK
- ThP 058 **Longitudinal Profiling of Type 1 Diabetes Human Plasma Using TMT10-based Quantitative Proteomics Approach**; Chih-Wei Liu¹; Lisa Bramer²; Bobbie-Jo Webb-Robertson²; Kathleen Waugh³; Marian J Rewers³; Qibin Zhang¹; ¹University of North Carolina at Greensboro, Greensboro, NC; ²Pacific Northwest National Laboratory, Richland, WA; ³University of Colorado School of Medicine, Aurora, CO

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- ThP 060 **A Validated Multiplex Assay for the Quantification of Tryptophan and Four of Its Catabolites in Human Plasma and Cerebrospinal Fluid;** Joachim Hoke¹; Andre Liesener²; Stefan Blech¹; ¹Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany; ²Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany
- ThP 061 **In vivo Metabolic Profiling of the TCA Cycle;** Stephanie Dale¹; Sheerin Shahidi-Latham¹; E. Ellen Jones¹; Cristine Quiason¹; ¹Genentech Inc, South San Francisco, CA
- ThP 062 **Comprehensive Profiling of Neurotransmitters in Cerebrospinal Fluid by LC-MS/MS;** Kanta Horie¹; Yoshiaki Sato¹; Takashi Kosasa¹; Takeyasu Tomioka¹; Motohiro Shiotani¹; Makoto Ogo¹; Yoshiya Oda²; ¹Eisai Co. Ltd., Tsukuba, Japan; ²Eisai Inc, Woodcliff Lake, NJ
- ThP 063 **Development of a Quantitative LC-MS Assay to Evaluate Depletion of Wall Teichoic Acid in Staphylococcus Aureus;** Olga Berejniaia; Merck & Co., Inc., Rahway, NJ
- ThP 064 **Validation of a High-Throughput Assay for the Quantification of Unbound and Total Desmosine and Isodesmosine in Human Plasma;** Andre Liesener¹; Joachim Hoke²; Stefan Blech²; ¹Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany; ²Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany
- ThP 065 **Rapid Quantitative Analysis of 15 Major Bile Acids in Human Serum by UPLC-Tandem Mass Spectrometry;** Tian-Sheng Lu¹; Aiping Zhu¹; Wanqing Lu¹; Emily Epure¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- ThP 066 **A Simultaneous Quantification Method of tricarboxylic Acid Cycle precursors and Intermediates;** Paul Rainville¹; Robert Plumb¹; Jose Castro-Perez¹; James Langridge¹; ¹Waters, Milford, MA
- ThP 067 **Challenges in Development of LC-MS Methods for Highly Polar, Low Molecular Weight Compounds: A Quantitative Assay for Quinolinic Acid;** Regina Oliveira¹; Asoka Ranasinghe¹; Joelle M Onorato¹; Celia D'Arienzo¹; Petia A Shipkova¹; ¹Bristol-Myers Squibb, Princeton, NJ
- ThP 068 **Development and Validation of a Method for the Determination of Total Plasma Cholesterol Levels to Support 4 β -Hydroxycholesterol Biomarker Studies;** Mark Leahy¹; Matt Byers¹; Victoria Jennings²; Joanne Hanson²; ¹Covance, Madison, WI; ²Covance, Harrogate, UK
- ThP 069 **Chiral Chromatography-Stable Isotope Dilution-Multiple Reaction Monitoring Mass Spectrometry for Characterization and Quantification of Complex Lipids in Human Biological Matrices;** Reza Nemat Josheghani¹; Christopher Dietz¹; Emily Anstadt²; Robert Clark²; Michael Michael Smith¹; Frank Nichols²; Xudong Yao¹; ¹University of Connecticut, Storrs, CT; ²University of Connecticut, Farmington, CT
- ThP 070 **Simultaneous Determination of Dehydroepiandrosterone (DHEA) and 17-Hydroxyprogesterone (17-OHP) in Human Plasma using LC-MS/MS;** Guangnong Zhang¹; Gaungchun Zhou¹; Feng Yin¹; Morgan Byrd¹; Tian-Sheng Lu¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- ThP 071 **Quantitative Analysis of Serum 2-Hydroxyglutarate using Gas Chromatography-Mass Spectrometry;** Salil Kumar Bhowmik^{1,2}; Nagireddy Putluri^{1,3}; Arun Sreekumar^{1,2,4}; ¹Dept. of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX; ²Alkek Center for Molecular Discovery, Baylor College of Medicine, Houston, TX; ³Advanced Technology Core, Baylor College of Medicine, Houston, TX; ⁴Verna and Marrs McLean Department of Biochemistry, Baylor College of Medicine, Houston, TX
- ThP 072 **Scaling Up: Improving Automated, High Throughput Measurement of Tobacco-Specific Nitrosamines in Urine by Liquid Chromatography-Atmospheric Pressure Ionization Tandem Mass Spectrometry;** Baoyun Xia¹; Christina R Brosius²; Yang Xia¹; Tonya Guillot¹; John Lee¹; Keegan J Nicodemus²; Dana Freeman²; Justin Lamar Brown²; Li Zhang³; Lanning Wang¹; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²ORISE Centers for Disease Control and Prevention, Atlanta, GA; ³Battelle Memorial Institute, Atlanta, GA
- ThP 073 **A Simple, Robust Method for Quantitative Analysis of Bile Acid Biomarkers in Human, Monkey, Dog, Mouse, and Rat Plasma Samples;** Angela Qi Shen¹; Alyssa Kabat¹; Wenlin Yuan¹; Ritika Kurian¹; Brittany Perley¹; Steven Wiltshire¹; ¹Agilux Laboratories, Worcester, MA
- ThP 074 **Quantitation of 2-Hydroxyglutarate and α -Ketoglutarate: Impact of Matrix Selection;** Vikki M Tsefrikas¹; Kyle S. Goodsell¹; Dylan S. Bennett¹; David Brigham¹; Allysen Meymaris¹; ¹Agilux Laboratories, Worcester, MA
- ThP 075 **Identification of Plasma Phospholipids that Distinguish Normal Subjects from Asthma Patients and Separating Patients of Lower Airway Diseases;** Hay-Yan J. Wang¹; Zhi-Fu Zheng²; Kuan-Lun Su²; Chau-Chyun Sheu³; Shau-Ku Huang⁴; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan; ²National Sun Yat-Sen University, Kaohsiung, Taiwan; ³Kaohsiung Medical University Hospital, Kaohsiung, Taiwan; ⁴National Health Research Institutes, Miaoli, Taiwan
- ThP 076 **Quantitation of the Organic Acid Biomarkers Pyruvate and Lactate in Biological Matrices;** Dylan Bennett¹; Allysen Meymaris¹; Vikki Tsefrikas¹; ¹Agilux Laboratories, Worcester, MA
- ThP 077 **Quantitative Analysis of Short Chain Fatty Acids and Ketone Bodies in Plasma and Tissues as Oximes Derivatives by LC-MS/MS;** Huachuan Marc Cao¹; Mingfei Zeng¹; ¹Eli Lilly and Company, Shanghai, China
- ThP 078 **Quantitation of (C22:6)-bis(monoacylglycerol) phosphate and Profiling of Additional BMPs in Rat Urine as Markers of Phospholipidosis;** Joelle Onorato¹; Petia Shipkova²; Mike Reily³; Yan He²; David Nelson²; Lois Lehman-McKeeman²; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb Co., Princeton, NJ; ³Bristol Myers Squibb, Princeton, NJ
- ThP 079 **Identification and Quantification Method for 2AG, 1AG and Arachidonic Acid in Plasma, CSF and Brain by LC-MS/MS;** Shakey Quazi; Pfizer, Andover, MA
- ThP 080 **Quantitative Analysis of D-Alanine in Cerebral Spinal Fluid Using a Chiral HPLC Coupled with High Resolution Mass Spectrometry;** Brendan Tierney¹; Christopher Holliman¹; Hongying Gao¹; ¹Pfizer, Inc., Groton, CT
- ThP 081 **High Throughput UPLC-MS/MS Method for the Profiling of 11 Hydrosoluble Vitamins in Human Plasma;** Oksana Lavrynenko¹; Serge Rezzi¹; ¹NIHS, Molecular Nutrition Group, Lausanne, CH
- ThP 082 **Detection of Aromatic Amines in Human Urine at ppt Level: a Semi-Automated Hamilton STAR/GC/MS/MS Method;** Tiffany Seyler¹; Elizabeth Cowan¹; Susan Pyatt²; Aaron Danberry³; Kyle Emer¹; ¹CDC, Atlanta, GA; ²Former Associate Fellow, Atlanta, GA; ³Former ORISE Fellow, Atlanta, GA
- ThP 083 **LC-MS/MS Quantitative Analysis of the Biomarkers Tryptophan, Kynurenine, and Kynurenic Acid in Mouse and Rat Plasma and Brain;** Alyssa Kabat¹; Brittany Perley¹; Steven Wiltshire¹; ¹Agilux Laboratories, Worcester, MA

- ThP 084 **Bioactivation of Heterocyclic Aromatic Amines by UDP Glucuronosyltransferases;** Tingting Cai¹; Lihua Yao¹; Robert Turesky¹; ¹University of Minnesota at Twin Cities, Minneapolis, MN
- ThP 085 **Urine Steroid Metabolite Profiling Using LC-HRMS for Diagnosing Adrenal Cortical Carcinoma;** Jolaine Hines¹; Irina Banocs¹; Robert L Taylor¹; Raman Deep Singh¹; Aditya V Avula¹; Stefan K Grebe¹; Ravinder J Singh¹; ¹Mayo Clinic, Rochester, MN
- ThP 086 **Quantification of Lathosterol in Human Plasma Using UPLC-MS/MS System;** Guangchun Zhou¹; Tian-Sheng Lu¹; Nicole Greer¹; Yong-Xi Li¹; ¹Medpace Bioanalytical Laboratories, Cincinnati, OH
- ThP 087 **Determination of Amino Acids and Biogenic Amines in Plasma and Urine in Cri Du Chat Disease by Mass Spectrometry;** Danielle Zildeana Furtado¹; Leticia Dias Lima Jedlicka¹; Heron Domingues Silva¹; Nilson Antonio Assunção^{1,2}; ¹UNIFESP, São Paulo, Brasil; ²The Scripps Research Institute, La Jolla, CA
- ThP 088 **Multiplex Quantitative Localized Analysis of Metal-Tagged Antibodies using Event-By-Event Cluster Secondary Ion Mass Spectrometry;** Dmitriy Verkhoturov¹; Kyungjin Son²; Stanislav V Verkhoturov¹; Michael J Eller¹; Alexander Revzin²; Emile A Schweikert¹; ¹Texas A&M University, College Station, TX; ²University of California-Davis, Davis, CA
- ThP 089 **Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA;** Ignacio Ortea¹; Michael Blank²; Romain Huguet²; David M Horn²; Daniel Lopez Ferrer³; Andreas Huhmer²; ¹IMIBIC, Cordoba, Spain; ²Thermo Fisher Scientific, San Jose, CA; ³ThermoFisher, Palo Alto, CA

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- ThP 090 **Anti-Cancer Drug Detection at the Single Cell Level;** Shawna Standke¹; Ning Pan¹; Naga Rama Kothapalli¹; Zhibo Yang¹; Anthony W. Burgett¹; ¹University of Oklahoma, Dept. of Chem & Biochem Norman, OK
- ThP 091 **Comparative Studies on Intrinsic Clearance Predication of Low Turnover Compounds Using the Regular and Relay Cryopreserved Hepatocyte Methods;** Min Jiang¹; Zhican Wang²; Dan Rock²; ¹Amgen, South San Francisco, CA; ²Amgen, Inc. South San Francisco, CA
- ThP 092 **Evaluation of QTOF HRMS Platform for Highly Sensitive Analysis of Raltegravir in Plasma in Support of Human Microdosing;** Li Sun¹; Kevin Bateman¹; Sukhdev Bangar²; Yun W Alelyunas³; Mark Wrona³; Sheila Breidinger¹; Eric Woolf¹; ¹Merck & Co., Inc., West Point, PA; ²Waters Corporation, Beverly, MA; ³Waters, Milford, MA
- ThP 093 **Characterization of Ketamine Metabolism in Liver S9 Fractions from Aging Sprague Dawley Rats by Liquid Chromatography Tandem Mass Spectrometry;** Raphaël Santamaria¹; Marie-Chantal Giroux¹; Pascal Vachon¹; Francis Beaudry¹; ¹Université de Montréal, St-Hyacinthe, QC
- ThP 094 **Methods for Analysis of Hydroxywarfarin Regio- and Stereoisomers in Bioanalytical Samples;** Karin Keller¹; Laura Drake¹; Crystal D Sergeant¹; Edward Wells¹; Steve E Unger¹; ¹Worldwide Clinical Trials, Austin, TX
- ThP 095 **Determination of Cariprazine and Metabolites in Human Plasma by LC-MS/MS;** Jing Ke¹; Guiyan Chen¹; Allan Xu¹; ¹Keystone Bioanalytical Inc, North Wales, PA
- ThP 096 **Characterization of clozapine-N-oxide using LC-MS/MS;** Jeffrey F Kuhn¹; Yu-wei Chen¹; Patricia Jensen¹; Leesa Deterding¹; ¹NIEHS, RTP, NC
- ThP 097 **Development and Validation of a Novel Enzyme Inhibition Assay for Determination of Statin Acid in Human Plasma using LC-MS/MS;** Yanjun Hu¹; Huafang Jiang¹; Junxian Zhao²; Wanhui Liu²; Xinping Fang¹; Xin Zhang¹; Wenzhong Liang³; ¹WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China; ²Luye Pharma Group Co., Ltd, Yantai, China; ³WuXi AppTec (Shanghai) Co. Ltd., Shanghai, Shanghai
- ThP 098 **Development and Validation of the Determination of Total CRS3123 in Human Urine by High Performance Liquid Chromatography Tandem Mass Spectrometry;** X. Steven Yan¹; Marsha L. Luna¹; ChenYu Chung¹; Julie Showalter¹; Yansheng Liu¹; Matthew E Hinz²; ¹KCAS Bioanalytical & Biomarker Services, Shawnee, KS; ²DynPort Vaccine Company, Frederick, MD
- ThP 099 **LC-MS/MS Method for the Quantification of Fingolimod and Fingolimod Phosphate in Rat blood with Storage Stability;** Rajesh Kumar Boggavarapu¹; Nagasurya Prakash Padala¹; Praveen kunduru¹; Devender Reddy Ajjala¹; Ramakrishna Nirogi¹; ¹Suven Life Sciences Ltd, Hyderabad, Telangana
- ThP 100 **Testing the Ability of UBP-310 to Diffuse into Mouse Brain via LC-MS/MS (QQQ) Quantification;** Sandy Stayte¹; Russell Pickford²; Justin Nash¹; Bryce Vissel¹; ¹Garvan Institute, Sydney, Australia; ²University of New South Wales, Sydney, Australia
- ThP 101 **Solving the Enigma of Nitrate Tolerance with a Stable Isotope-Assisted, Multi-Platform Work Flow;** Elizabeth Axton¹; Eleonso Cristobal¹; Fred Stevens¹; ¹Oregon State University, Corvallis, OR
- ThP 102 **Using Triplicate Calibration Curves and Weighted Least Squares Regression to Reduce Experimental Error;** Kenneth Anderson¹; Kevin P Bateman²; ¹Merck & Co, Inc., West Point, PA; ²Merck & Co., Inc., West Point, PA
- ThP 103 **Systematic Investigation of the Failure of One Analyte during Method Transfer and Cross Check of a 4-in-1 LC-MS/MS Method;** Bian Chao¹; Daniel Neddermann²; Lihua Qiao¹; Yixin Yang¹; Liang Wenzhong¹; Xin Zhang¹; ¹WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China; ²Novartis Pharma AG, Basel, Switzerland
- ThP 104 **Ionization Efficiency of Oligopeptides and Small Hydrophilic Molecules in ESI/MS;** Piia Liigand¹; Karl Kaupmees¹; Anneli Kruev¹; ¹University of Tartu, Institute of Chemistry, Tartu, Estonia
- ThP 105 **In-vitro Metabolic Stability and Profiling of Ponatinib, Vandetanib and Masitinib using Liquid Chromatography Tandem Mass Spectrometry;** Sawsan M Amer¹; Adnan A. Kadi²; Hany W Darwish^{1,2}; Mohamed W. Attwa^{1,2}; ¹College of Pharmacy, Cairo University Cairo, Egypt; ²College of Pharmacy, King Saud University Riyadh, Saudi Arabia
- ThP 106 **Unusual Matrix Effects Observed during Quantitative LC-MS/MS Methods Development;** Yuyong ke¹; Nicki Hughes^{1,2}; Fernand Labrie²; ¹Bioanalytical Laboratory Services, a Division of LifeLabs LP, Toronto, Ontario; ²EndoCeutics, Quebec City, QC
- ThP 107 **Evolution, Development, and Application of a Dynamic, High-Throughput, Enterprise-Level Autosampler for High-Performance LC/MS/MS Bioanalysis;** Brendon Kapinos¹; John S Janiszewski¹; Hui Zhang¹; Mary Piotrowski¹; Jianhua Liu¹; Wayne Lootsma²; Steven Ainley²; ¹Pfizer, Groton, CT; ²Sound Analytics, Niantic, CT

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- ThP 109 **A Multi-Residue Liquid Chromatography/Tandem Mass Spectrometry Method for the Analysis of Macrolides in Food Matrices;** Pavel Metalnikov¹; Iliia Batov²; Renat

- Selimov²; Ksenia Batova²; Alexander Komarov²; ¹VGNKI, Moscow, Moscow; ²VGNKI, Moscow, Moscow
- ThP 110 **Determination of Wilfordine and Wilforine in Honey using Liquid Chromatography with Tandem Mass Spectrometry**; Chen Jianli; Shimadzu, Wuhan, China
- ThP 111 **Determination and Quantification of Perchlorate in a Fruit Matrix Using Accelerated Solvent Extraction and IC-MS**; Kyle Renfrew; Amanda Hartman¹; Nicholas Santiago; ¹Thermo Fisher Scientific, Austin, TX
- ThP 112 **Determination of Papaverine and Other Alkaloids in Hot Pot Condiment by Direct Analysis in Real Time Mass Spectrometry**; Yi Li¹; Weixia Wang¹; Xiaohui Xiong¹; Jiehui Hu²; Charles C. Liu²; ¹Nanjing Tech University, Nanjing, Jiangsu; ²ASPEC Technologies Limited, Beijing, Beijing
- ThP 113 **Use of Ambient Ionization Mass Spectrometry for the Rapid Authentication of Food and Dietary Supplements**; Kari Organtini¹; Gareth Cleland¹; Beth Loecken¹; Adam Ladak¹; ¹Waters, Milford, MA
- ThP 114 **Accessible and Efficient Screening of Multiclass Contaminants in Food**; Eimear McCall¹; Ramesh Rao¹; Adam Ladak²; Jennifer Burgess²; ¹Waters, Wilmslow, UK; ²Waters, Milford, MA
- ThP 115 **Authentication and Chemical Standardization of Licorice Dietary Supplements Using UHPLC-MS/MS**; Guannan Li^{1,2}; Charlotte Simmler^{1,2}; Dejan Nikolic^{1,2}; Shao-Nong Chen^{1,2}; Guido F. Pauli^{1,2}; Richard B. van Breemen^{1,2}; ¹UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL; ²Department of Medicinal Chemistry and Pharmacognosy, University of Illinois College of Pharmacy, Chicago, IL
- ThP 116 **Analysis of Phosphodiesterase Type 5 Inhibitors Extracted from Herbal Preparations by DSA-TOF MS**; Robert J. Seward¹; Jason Weisenseel¹; Craig Young¹; Wilhad M. Reuter¹; ¹PerkinElmer, Waltham, MA
- ThP 117 **Simultaneous Determination of Multiple Plant Growth Regulators in Bean Sprouts using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Cheng Zheng¹; Qiaoyuan Cheng¹; Weifang Ni¹; Chengyuan Cai²; Jingchao Lin²; Yongming Xie²; ¹Zhejiang Institute of Food and Drug Control, Hangzhou, China; ²PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China
- ThP 118 **High Sensitive Analysis of Peanut Allergen in Cumin and Spice Mix**; Clifford Robert¹; Tairo Ogura¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- ThP 119 **Simultaneous Determination of Hormones in Edible Bird's Nest using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Dunming Xu¹; Liping Zhong¹; Sanmei Zeng¹; Lizhong Yang²; Chengyuan Cai²; Jingchao Lin²; Yongming Xie²; ¹Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; ²PerkinElmer Management(Shanghai)Co., Ltd, Shanghai, China
- ThP 120 **Mass Spectrometry Based Methods to Detect the BoNTE in Catfish Specimen**; Tibor Pechan¹; Olga Pechanova²; Jennifer Arnold³; ¹Mississippi State University, Mississippi State, MS; ²Mississippi State University, Starkville, MS; ³Edward Via College of Osteopathic Medicine - Carolinas Department of Biomedical Science, Spartanburg, SC
- ThP 121 **Rapid Screening and Quantitation of Domoic Acid in Shellfish Homogenates using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS)**; Pamela S. Cantrell¹; Callee M. Walsh²; Haddon E. Goodman²; Pearse McCarron³; Kelley Reeves³; Wade A. Rourke⁴; Sinead O'Brien⁵; Daniel G. Beach³; ¹Protea Biosciences, Morgantown, WV; ²Protea Biosciences, Inc. Morgantown, WV; ³National Research Council Canada, Halifax, Nova Scotia, Canada; ⁴Canadian Food Inspection Agency, Dartmouth, Nova Scotia, Canada; ⁵Marine Institute, Galway, Ireland
- ThP 122 **Analysis of Diarrhetic Shellfish Poisoning and Azaspiracid Shellfish Poisoning Toxins by Liquid Chromatography-Tandem Mass Spectrometry**; Li Yang¹; Randy Self¹; James Stuart¹; Theodore Lapainis¹; Daniel Rice¹; Wen-Hsin Wu¹; James Hungerford¹; ¹Food and Drug Administration, Bothell, WA
- ThP 123 **Multi-analyte Investigation in Relation to the Illicit Treatment of Fish Food with Hydrogen Peroxide**; Claudio Medana¹; Riccardo Aigotti¹; Federica Dal Bello¹; Valentina Santoro¹; Claudio Baiocchi¹; ¹University of Turin, Torino, Italy
- ThP 124 **Origin Determination of Eastern Oyster (Crassostrea virginica) by Combination of Heavy Metal Concentrations, Whole-Body Bulk and Compound Specific Isotope Analyses**; Mayara P. V. Matos¹; Marc E Engel²; Glen P Jackson^{3,4}; ¹Department of Biology, West Virginia University, Morgantown, WV; ²Florida Department of Agriculture and Consumer Service, Tallahassee, FL; ³Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; ⁴C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV
- ThP 125 **Quantitative Determination of Veterinary Drug Residues in Eggs by UPLC-MS/MS Using a Simple, Rapid and Effective Cleanup Approach**; Sujie Xia¹; Dimple Shah²; Jeremy C Shia²; Michael S Young²; Adam Ladak²; Laura Suhadolnik²; ¹Shanghai Institute for Food and Drug Control, Shanghai, China; ²Waters, Milford, MA
- ThP 126 **Targeted Veterinary Drugs Screening in Food Matrix using EMR QuEChERS and Newly Developed Triple Quadrupole Mass Spectrometer**; Yanan Yang¹; Dan-Hui Yang²; ¹Agilent Technologies, Inc, Santa Clara, CA; ²Agilent Technologies, Santa Clara, CA
- ThP 127 **Development of Multi-Class, Multi-Residue UHPLC MS/MS Method for Screening/Quantification of Veterinary Drugs in Complex Food Matrices and Related Products**; Azeem Hasan¹; Hui Zhao¹; John Zulkoski¹; Barb Mitchell¹; Thomas Vennard¹; Katerina Mastovska¹; ¹Covance, Madison, WI
- ThP 128 **Extending the Linear Dynamic Range for Measurements Targeting Veterinary Drug Residues in Animal Feed by UPLC-laminar Flow HSID-MS/MS**; Jason Kong¹; Frank Kero²; Joshua Ye³; Lisa Cousins³; Craig Young²; Sharanya Reddy²; ¹Ohio Department of Agriculture, Reynoldsburg, OH; ²PerkinElmer, Shelton, CT; ³Ionics Mass Spectrometry Group, Bolton, Canada
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- ThP 130 **Meat Species Identification by Protein Profiling and Spectral Fingerprinting using MALDI-TOF-MS**; Man On So; ¹The Hong Kong University of Science and Technology, Hong Kong SAR, HK
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- ThP 146 **Substance Characterization of Polyethylene Polyamine by EI GC/MS;** O. David Sparkman¹; Kirill Tretiyakov²; Patrick Batton³; Itsuko Iwai Iwai⁴; Terry L. Ramus⁴; ¹University of the Pacific, Antioch, CA; ²Dakota Consulting Inc., Silver Springs, MD; ³University of the Pacific, Stockton, CA; ⁴Diablo Analytical, Antioch, CA
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- ThP 198 **MALDI-MSI for the Study of Flow-Cell and Agar Bound Microbial Biofilms;** Bin Li¹; Sage Dunham²; Tong Si²; Ning Yang²; Clint Arnett³; Sweedler Jonathan²; ¹University of Illinois at Urbana-Champaign, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ³Engineer Research and Development Center-Construction Engineering Research Laboratory (ERDC-CERL), Champaign, IL

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- ThP 204 **Quantitative MALDI-MS Imaging of Tumour Spheroids**; Rebecca Day¹; Laura Cole¹; Ieva Palubeckaitė¹; David Smith¹; Neil Cross¹; Malcolm R Clench¹; ¹Sheffield Hallam University, Sheffield, UK
- ThP 205 **MALDI Directed – Infrared Laser Ablation Sample Transfer for Spatially Resolved Biomolecule Analysis**; Kelin Wang¹; Fabrizio Donnarumma¹; Kermit K Murray¹; ¹Louisiana State University, Baton Rouge, LA
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¹University of Alabama at Birmingham, Birmingham, AL;

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- ThP 471 **Selenium Labeling Combined with LC-ICP-MS, a New Methodology in Pharmacology to Measure Protein-Ligand Interactions**; Emmanuelle Cordeau¹; Carine Arnaudguilhem²; Brice Bouyssié²; Agnès Hagège³; Jean Martinez¹; Gilles Subra¹; Sonia Cantel¹; Christine Enjalbal¹; ¹Institut des Biomolécules Max Mousseron (IBMM), UMR 5247, Université de Montpellier, CNRS, ENSCM, Place Eugène Bataillon, 34095 Montpellier cedex 5, France.; Montpellier, France; ²Laboratoire de Chimie Analytique Bio-inorganique et Environnement LCABIE-IPREM, UMR 5254, Hélioparc, 64053 Pau, France, Pau, France; ³Université de Lyon, Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1, ENS Lyon, Villeurbanne, France, Lyon, France
- ThP 472 **Development of a Robust GLP Bioanalytical Method for a Short-lived Therapeutic Peptide**; Christopher Barringer¹; Daniel J Ricca²; Mary Katofiasc²; Lesley Marson²; ¹Covance, Durham, NC; ²Dignify Therapeutics, Research Triangle Park, NC
- ThP 473 **An Alternative and More Sensitive Approach for the Analysis of Neuropeptides in Biological Samples**; Stephen J. Lock¹; Edna Betgovarguez²; ¹SCIEX, Warrington, Cheshire; ²SCIEX, Concord ON, Canada
- ThP 474 **Development of a MicroFlow LC-MS/MS Method for Quantitation of Peptides**; Kerry Hassell¹; Joshua J Nicklay¹; Tara Schroeder¹; ¹ThermoFisher Scientific, Somerset, NJ
- ThP 475 **A Simplified Approach to Fast and Accurate, High Throughput Targeted MS2 Quantitation using Internal Standards**; Shannon Eliuk¹; Romain Huguet¹; Michael Blank¹; Vlad Zabrouskov¹; Graeme C McAlister¹; ¹Thermo Fisher Scientific, San Jose, CA
- ThP 476 **Validation and Correlation Strategies for Data Generated by Ligand Binding Assays and LC-MS to Support Product Development and Regulatory Assessment**; Ryan Hill¹; Trent J. Oman¹; ¹Dow AgroSciences, Indianapolis, IN
- ThP 477 **Novel Application of SCIEX 6600 TripleTOF Mass Spectrometer for Quantitative Assessment of Glucagon-Like Peptide-1 (GLP1) Analog Pharmacokinetic Studies**; Yue Huang¹; Sarah Will²; Anish Konkar²; Jefferson Revell³; Marcella Petrone³; Inna Vainshtein¹; Meina Liang¹; Raffaella Faggioni¹; Anton Rosenbaum¹; ¹MedImmune, Mountain View, CA; ²MedImmune, Gaithersburg, MD; ³MedImmune, Cambridge, UK
- ThP 478 **Effect of Dimethyl Sulfoxide on Sensitivity Improvement of Therapeutic Peptides by LC/MS/MS**; Eric Ma¹; Moucun Yuan¹; William Mylott¹; Bruce Hidy¹; Rand Jenkins¹; ¹PPD, Richmond, VA
- ThP 479 **Improvements in Sensitivity for Biotherapeutics using a Prototype Tandem Quadrupole Mass Spectrometer**; Nikunj Tanna¹; Kerri Smith¹; Mark Wrona¹; Leonard Dillon²; Mark Roberts²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, UK
- ThP 480 **Peakjuggler – A Proteome Discoverer Node for Label-free MS1 Quantification**; Johannes Doblmann¹; Karl Mechtler^{1,2}; ¹Research Institute of Molecular Pathology (IMP), Vienna, Austria; ²Institute of Molecular Biotechnology (IMBA), Vienna, Austria
- ThP 481 **Evaluation of the Parameters Affecting Interference Levels in Isobaric Tagging Studies**; Matthew Lim¹; Joao Paulo¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA
- ThP 482 **Relative Quantification of Sites of Peptide and Protein Modification using Size Exclusion Chromatography coupled with Electron Transfer Dissociation**; Boer Xie¹; Joshua Sharp²; ¹The University of Georgia, Athens, GA; ²The University of Mississippi, Oxford, MS
- ThP 483 **Quantification of Total Hepatocyte-Targeted Membrane-Lytic-Peptide (MLP-NAG) in Rat Plasma by LC-MS/MS using Solid Phase Extraction**; Qingguo Tian¹; Min Meng²; Rogness Juan³; Zhen Li⁴; ¹Arrowhead Research Corporation, Madison, WI; ²Covance, Salt Lake City, UT; ³Covance, Salt Lake City, UT; ⁴Arrowhead Research Corporation, Madison, WI
- ThP 484 **MALDI Mass Spectrometry and HCCA Labeling as a Powerful Tool for Peptide Quantitation in Biology**; Christine Enjalbal¹; Maxime Rossato²; Sonia Cantel²; Gilles Subra²; Muriel Amblard²; Jean Martinez²; ¹University Montpellier 2, Montpellier, cedex 05; ²University of Montpellier, IBMM UMR5247, Montpellier, France
- ThP 485 **Extending Targeted Proteomics to Study Molecular Signaling Events**; Thierry Schmidlin^{1,2}; Luc Garrigues^{1,2}; Violette Gautier^{1,2}; Arjen J. Boender¹; Erik L de Graaf^{1,2}; Roger A H Adan¹; Albert J R Heck^{1,2}; Maarten A F Altelaa^{1,2}; ¹Utrecht University, Utrecht, The Netherlands; ²Netherlands Proteomics Center, Utrecht, The Netherlands
- ThP 486 **Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Human Uterine Smooth Muscle in Disparate States of Pregnancy**; Christian Copley Salem¹; Crag Ulrich¹; David Quilici²; Rebekah Woosley²; Iain Buxton¹; Heather Burkin¹; ¹University of Nevada, Reno School of Medicine, Reno, NV; ²Mick Hitchcock Nevada Proteomics Center, Reno, NV
- ThP 487 **Quantification of Synthetic Peptides by Multiple Reaction Monitoring-Liquid Chromatography-Mass Spectrometry (MRM-LC-MS)**; Praveena Nukareddy¹; Bruce O'Rourke¹; Dwight E. Matthews¹; ¹University of Vermont, Burlington, VT
- ThP 488 **Precise and High-Throughput Quantitation of Plasma Biomarker Peptides for Alzheimer Disease at Attomole Level by SRM**; Takeshi Tomonaga¹; Ritsuko Maki¹; Kanta Yanagida²; Shigeru Yamada³; Shinji Tagami²; Masayasu



- Okochi²; ¹Laboratory of Proteome Research, National Institutes of Biomedical Innovation, Health and Nutrition, Osaka, Japan; ²Psychiatry, Department of Integrated Medicine, Division of Internal Medicine, Osaka University Graduate School of Medicine, Osaka, Japan; ³Thermo Fisher Scientific Japan, Yokohama, Japan
- ThP 489 **A High-Throughput Method for Reproducible Global Quantification of the Yeast Proteome using Data Independent Acquisition Mass Spectrometry;** Lindsay Pino¹; Jennifer E Merrihew¹; William S Noble¹; Michael J MacCoss¹; ¹University of Washington, Seattle, WA
- ThP 490 **Fast and Sensitive LC-MS Workflow for Determination of Endogenous Secretory Peptides in Biological Fluids;** Liangqiao Bian¹; Maciej Kukula²; ¹SCAAC, UT Arlington, Arlington, TX; ²SCAAC, University of Texas at Arlington arlington, tx
- ThP 491 **Quantitative Analyses of Microcystins by LC-MS/MS using an Orbitrap Fusion Tribrid Mass Spectrometer;** Raymond West¹; Dilrukshika S.W. Palagama¹; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH
- ThP 492 **Label-free Quantitation of Opioid Induced Hyperalgesia Related-Peptides in Mice Hypothalamus using Skyline MS1 Filtering Approach;** Ning Yang¹; Krishna D Anapindi¹; Stanislav S Rubakhin¹; Elena V Romanova¹; Amynah Pradhan²; Jonathan v Sweedler¹; ¹University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ²University of Illinois at Chicago, Chicago, IL
- ThP 493 **Characterization of Endoproteolytic Processing of Tachykinins and Substance P using Mouse Spinal Cord Cellular Fractions and High-Resolution Mass Spectrometry;** Mouna Saidi¹; Francis Beaudry¹; ¹Université de Montréal, St-Hyacinthe, QC
- ThP 494 **Selective and Sensitive Quantification of Glucagon and Glucagon-Related Peptide Hormones in Human Plasma using Conventional LC/MS/MS;** Norihide Yokoi¹; Ritsuko Hoshikawa¹; Toshiya Matsubara^{1,2}; Ichiro Hirano²; Susumu Seino¹; ¹Kobe University Graduate School of Medicine, Kobe, Japan; ²Shimadzu Corporation, Kyoto, Japan
- ThP 495 **Quantification of Blood-Brain Barrier Permeation of Glycosylated Peptides using Microdialysis Coupled to Mass Spectrometric Detection;** Catherine Kramer¹; Evan M. Jones¹; Meredith Hay¹; Robin Polt¹; Michael L Heien¹; ¹University of Arizona, Tucson, AZ
- ThP 496 **Ultra Performance Liquid Chromatography-Tandem Quadrupole Mass Spectrometry for High-Sensitivity Profile Analysis of Blood Pressure Modulators Angiotensin Peptides;** Meng Qi¹; Hui Wang²; Jie Wang¹; Li Yang¹; Zhengtao Wang¹; ¹Shanghai University of Traditional Chinese Medicine, Shanghai, Shanghai; ²Waters Corporation, Shanghai, China
- ThP 497 **Detection of Insulin Analogues and Large Peptides in Urine for Anti-doping;** Holly Cox¹; Brittney Weber¹; Daniel Eichner¹; ¹Sports Medicine Research and Testing Laboratory, Salt Lake City, UT
- ThP 498 **Validation of Vancomycin Assay in Rat Plasma by Liquid Chromatography /Tandem Mass Spectrometry;** Xiaodong Shen¹; Chantal Picard¹; Rwaidda Al-Eryani¹; John Lord²; Gary Johnson¹; ¹ITR, Baie d'Urfe, Canada; ²Savara Inc., Austin, USA
- ThP 499 **Screening of Glyphosate-Resistant Transgenic Engineering Soy Bean and Maize by Ultra-high Performance Liquid Chromatography Coupled with Tandem Mass Spectrometry;** Wenjuan Zang¹; Meiling Lu²; Shan Zhou³; Xiangmin Zhang¹; ¹Fudan University, Shanghai, China; ²Agilent Technologies (China) Limited, Beijing; ³Agilent Technologies (China) Limited, Beijing, China
- ThP 500 **Systematic Comparison of TMT10-plex Quantification Accuracy and Precision in MS2 and SPS-MS3 Mode;** Lauren Clarissa Tang¹; Jana W Qiao¹; Rushdy Ahmad¹; Karl R Clauser¹; Namrata D Udeshi¹; Hasmik Keshishian¹; Caitlin Feeney¹; Jenn Abelin¹; Jacob J Jaffe¹; Philipp Mertins¹; Steven A Carr¹; ¹The Broad Institute, Cambridge, MA
- ThP 501 **One and Done - HRAM MS Protein Quantitation and the Rewards of Retrospective Data Analysis in an Ever-changing Regulatory Landscape;** Trent J Oman¹; Ryan C Hill¹; Jeffrey R Gilbert¹; ¹Dow AgroSciences, Indianapolis, IN
- ThP 502 **PTM Quantitative Analysis on Monoclonal Antibodies using LC-MS and PEAKS Software;** Baozhen Shan¹; Xin Lei²; ¹Bioinformatics Solutions Inc., Waterloo, ON; ²Bioinformatics Solutions Inc., Waterloo, Canada
- ThP 503 **The Myocardial Degradome following Ischemia/Reperfusion Injury;** Melanie Yvonne White¹; Nina Hartcher¹; Kiersten A Liddy¹; Joel A Cain¹; Stuart J Cordwell¹; ¹The University of Sydney, Sydney, Australia
- ThP 504 **Charge Variant Identification and Quantification of Recombinant Antibody, Trastuzumab Using Automated Software;** Jung-Keun Suh¹; Kui Hyun Kang²; John St Skilton³; Eric Carlson⁴; Chris Becker⁴; ¹Korean German Institute of Technology, Seoul, Gangseo-gu; ²BIONSYSTEMS Inc., Seoul, Korea; ³Protein Metrics Inc., San Carlos, CA; ⁴Protein Metrics, San Carlos, CA
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- ThP 505 **LC-MS/MS – Peptide Mapping with Electron Transfer Dissociation (ETD) Reveals Enzyme-Mediated Intramolecular Bond in Transglutaminase;** Thomas W Powers¹; Andrew W Dawdy¹; Jason C Rouse²; Olga V Friese¹; ¹Pfizer, Inc. Chesterfield, MO; ²Pfizer, Inc. Andover, MA
- ThP 506 **Heavyweight Champion: Iodine's Large Mass-Defect Weighs in on the Enhancement of the Sequence Coverage of Tryptic Peptides via ETD;** Emilie Aude Viglino¹; Christopher Shaffer¹; František Tureček¹; ¹University of Washington, Seattle, WA
- ThP 507 **Electron Transfer Dissociation of Trivalent Metal Cationized Acidic Phosphorylated Peptides;** Juliette Joan Commodore¹; Carolyn J. Cassidy¹; ¹The University of Alabama, Tuscaloosa, AL
- ThP 508 **Comparative Study of The Skin peptidomes of Rana ridibunda from Russian and Slovenian Populations;** Tatiana Yu Samgina¹; Konstantin A Artemenko²; Jonas Bergquist³; Polonca Trebse⁴; Gregor Torkar⁴; Maria Tolpina¹; Albert T. Lebedev⁵; ¹Moscow State University, Moscow, Russia; ²Uppsala University, Uppsala, SE; ³Uppsala University, Uppsala, Sweden; ⁴Ljubljana University, Ljubljana, Slovenia; ⁵Moscow State University, Moscow, Moscow
- ThP 509 **Sensitive and Rapid LC/MS Method to Identify Potential T-cell Epitopes of Antibody Drugs;** Nobuo Sekiguchi¹; Chiyomi Kubo¹; Ayako Takahashi¹; Kumiko Muraoka¹; Akira Takeiri¹; Mariko Yano¹; Shotaro Takata¹; Naoki Murao¹; Masaki Ishigai¹; ¹Chugai Pharmaceutical Co., Ltd., Gotemba, Shizuoka
- ThP 510 **Complete Sequence Coverage via ECD in a Q-ToF versus ETD/CID/HCD in an Orbitrap of 6+ and 7+ Protonated Ubiquitin;** Yury V Vasil'ev¹; Nathan I Lopez¹; Valery G Voinov¹; Douglas F Barofsky²; Joseph S Beckman¹; ¹Linus Pauling Institute, Oregon State University Corvallis, OR; ²Oregon State University, Department of Chemistry Corvallis, OR
- ThP 511 **Highly Specific Peptide-Bond Dissociation of Some Peptide Model Molecules;** Chen-Lin Liu; NSRRC, Hsinchu, Hsinchu
- ThP 512 **De novo Sequencing of Novel Antimicrobial Peptides from the Venom of the Scorpion *Isometrus maculatus* using ASDf-incorporated Curved Field Reflectron.;** Yuzo Yamazaki¹; Atsushi Kitanaka²; Mao Yakio²; Masahiro Miyashita³; Hisashi Miyagawa³; ¹Shimadzu Corporation, Kyoto, Japan; ²Graduate School of Agriculture, Kyoto

- University Kyoto, Japan; ³Graduate School of Agriculture, Kyoto University, Kyoto, Japan
- ThP 513 **Compact Mass Spectrometry (CMS) for Reaction Optimization and Quality Control of Modern Solid Phase Synthesis (SPPS) of Biologically Active Peptides;** Simon J. Prosser¹; Daniel Eikel¹; James P. Cain²; Elizabeth Restituyo-Rosario²; ¹Advion, Inc. Ithaca, NY; ²Protein Technologies Inc., Tucson, AZ
- ThP 514 **3-Hydroxy-4-nitrobenzoic Acid (3H4NBA) as a MALDI Matrix for In-Source Decay;** Yuko Fukuyama¹; Shunsuke Izumi²; Koichi Tanaka³; ¹Shimadzu Corporation, Kyoto; ²Hiroshima University, Higashi-Hiroshima, Japan; ³Shimadzu Corporation, Kyoto, Japan
- ThP 515 **Application of Hydrogen Attachment/Abstraction Dissociation (HAD) for Peptide Analysis;** Sadanori Sekiya¹; Hidenori Takahashi¹; Takashi Nishikaze¹; Shosei Yamauchi¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 516 **Selective Derivatization of Peptide Carboxyl Groups with Fluorophores for LDI-MS Analyses;** Dilrukshika S. W. Palagama¹; Raymond E. West III¹; Dragan Isailovic¹; ¹The University of Toledo, Toledo, OH
- ThP 517 **Elucidating the Mechanism of Photo-Induced Peptide Cleavage by Uranyl using Mass Spectrometry;** Rasmus Elnegaard¹; Niels Erik Møllegaard²; Thomas J. D. Jørgensen¹; Frank Kjeldsen¹; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; ²Department of Cellular and Molecular Medicine, University of Copenhagen, Copenhagen, Denmark
- ThP 518 **Fragmentation of Model Deprotonated Phosphorylated Peptides by Collision-Induced Dissociation;** Chelsea E. Plummer¹; Suma Kavati¹; Junjie Gao¹; Carolyn J. Cassidy¹; ¹The University of Alabama, Tuscaloosa, AL
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- ThP 519 **Comparing Mass Spectrometric Platforms for Neuropeptide and Neuroproteome Discovery from Well-Defined Neuronal Tissue;** Krishna D.B. Anapindi¹; Elena V. Romanova^{2,3}; Bruce R. Southey²; Jonathan V. Sweedler²; ¹University of Illinois-Urbana Champaign, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ³Beckman Institute, UIUC Urbana, IL
- ThP 520 **Correlating Differential Peptidomics and Transcriptomics Data for Assessing Seasonal Changes in the Camel Brain;** Elena Romanova¹; Bruce R. Southey¹; Michael Greenwood²; Charles Hindmarch³; Yea-Ling Tay⁴; Ahmad Yamin bin Abdul Rahman⁴; Kok-Gan Chan⁵; Mark Rogers²; Colin Campbell²; F. Zahra Djazouli Alim⁶; David Murphy²; Jonathan V. Sweedler¹; ¹University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; ²University of Bristol, Bristol, UK; ³Queen's University, Kingston, Canada; ⁴BioEasy Sdn Bhd, Shah Alam, Selangor Darul Ehsan, Malaysia; ⁵University of Malaya, Kuala Lumpur, Malaysia; ⁶Université Saad Dahlab de Blida, Blida, Algeria
- ThP 521 **Multifaceted Mass Spectrometric Investigation of Neuropeptide Changes in Blue Crab, Callinectes sapidus, in Response to Ocean Acidification;** Yang Liu¹; Amanda Buchberger¹; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin, Madison, WI; ²School of Pharmacy, University of Wisconsin, Madison, WI
- ThP 522 **Mass Spectrometric Quantification and Imaging of Changes in Crustacean Neuropeptide Expression Levels Resulting from Hypoxia Stress;** Kellen DeLaney¹; Amanda Buchberger¹; Yang Liu¹; Lingjun Li¹; ¹UW Madison, Madison, WI
- ThP 523 **A Puzzle Approach on Single Cell Level;** Susanne Neupert; Biocenter Cologne, University of Cologne 50674 Cologne, Germany
- ThP 524 **Large Scale Discovery and de novo-Assisted Sequencing of Native Cationic Antimicrobial Peptides (CAMPs) from the Komodo Dragon (Varanus komodoensis);** Paul Russo¹; Melanie Juba²; Megan Devine²; Stephanie Barksdale²; Kajal Gupta²; Shaylyn Scott²; Kent Vliet³; Joel Schnur²; Monique vanHoek²; Barney Bishop²; ¹George Mason University, Manassas, VA; ²George Mason University, Manassas, VA; ³University of Florida, Gainesville, FL
- ThP 525 **Immunogenic HLA-DR-presented-peptides Identified from Clinical Samples of Synovial Tissue/Fluid and Peripheral Blood from Patients with Rheumatoid Arthritis or Lyme Arthritis;** Qi Wang¹; Elise E. Drouin²; Chunxiang Yao¹; Jiyang Zhang¹; Yu Huang¹; Deborah R. Leon¹; Allen C. Steere²; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²Massachusetts General Hospital and Harvard Medical School, Boston, MA
- ThP 526 **Proto-Peptidomics: A UPLC-Ion Mobility-MS/MS Proteomics Workflow for Studying Early Peptide Evolution on the Prebiotic Earth;** Jay G. Forsythe^{1,2}; Anton S. Petrov^{1,2}; Sheng-Sheng Yu^{1,2}; W. Calvin Millar^{1,2}; Martha A. Grover^{1,2}; Ramanarayanan Krishnamurthy^{2,3}; Nicholas V. Hud^{1,2}; Facundo M. Fernandez^{1,2}; ¹Georgia Tech, Atlanta, GA; ²NSF/NASA Center for Chemical Evolution, Atlanta, GA; ³The Scripps Research Institute, La Jolla, CA
- ThP 527 **LC-MS-MS identification of Small Cyclic Amphipathic Peptides (SCampPs) in citrus phloem;** Leslie Harden¹; William H. Vensel²; Kent F. McCue²; William R. Belknap²; ¹USDA/WRRC, Albany, CA; ²U.S. Dept. of Agriculture, Albany, CA
- ThP 528 **Azoniaspiro[4.4]nonyl Scaffold for Quantitative Peptide Analysis by LC-ESI-MS/MS;** Bartosz Setner¹; Monika Kijewska¹; Alicja Kluczyk¹; Piotr Stefanowicz¹; Zbigniew Szewczuk¹; ¹Faculty of Chemistry, University of Wrocław, Wrocław, Poland
- ThP 529 **Electroanalysis and Electrospray Ionization Mass Spectrometry of Intact and Oxidized Hormone Glucagon;** Wendell P. Griffith¹; Sushma Karra¹; Robert Kennedy²; Waldemar Gorski¹; ¹University of Texas at San Antonio, San Antonio, TX; ²University of Michigan, Ann Arbor, MI
- ThP 530 **Proteomic Landscapes of Pachycondyla villosa Ant Venom by Nano-Scale Chromatography and High Resolution Mass Spectrometry;** Camilla Takeno Cologna¹; Loic Quinton¹; Edwin De Pauw¹; Michel Degueldre¹; ¹University of Liege, GIGA-Proteomics Liege, Belgium
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- ThP 531 **Profiling Released High Mannose and Complex N-Glycan Structures from Monoclonal Antibodies Using Optimized Hydr;** Scott McCall¹; Matthew Lauber¹; Stephan Koza¹; Erin Chambers¹; ¹Waters, Milford, MA
- ThP 532 **Comprehensively Characterizing the N and O-Linked Glycosylation of a Recombinant Human EPO using HILIC-MS;** Matthew Lauber¹; Stephan Koza¹; Erin Chambers¹; ¹Waters Corporation, Milford, MA
- ThP 533 **Mass Spectrometry Friendly Method for N-glycan Quantification;** Wei Wu¹; Jiping Zhou¹; Subbarao Mantha¹; Zhichao Fang¹; Michelle Wang¹; Li Tao¹; Tapan Das²; Reb Russell²; ¹Bristol-Myers Squibb Company, Bloomsbury, NJ; ²Bristol-Myers Squibb, Hopewell, NJ
- ThP 534 **Site-specific Characterization of N-/O- Glycosylation on Therapeutic Human Chorionic Gonadotropins using Online LC/MS and Tandem Mass Tags;** Hongbin Zhu¹; Ashley C. Ruth¹; David A. Keire¹; Hongping Ye¹; ¹FDA, St. Louis, MO

- ThP 535 **Substrate- and Substrate-mimetic Chaperone Binding Sites in Human Alpha-Galactosidase Revealed by Affinity- Mass Spectrometry;** Michael Przybylski¹; Stefan Maeser²; Adrian Moise²; Frederike Eggers²; Mary Murphy³; Jeff Bornheim³; ¹Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; ²Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; ³Reichert-Ametek Technologies, Buffalo, NY
- ThP 536 **Hydrogen Exchange Mass Spectrometry can Reliably Detect Small Fractions of Destabilized Protein in Comparability Studies;** Tyler Hageman¹; David D Weis¹; Jayant Arora¹; ¹University of Kansas, Lawrence, KS
- ThP 537 **Characterization of Bispecific Heteromab using LC-MS Based Methods;** Yuping Zhou¹; Jason Tang¹; ¹Eli Lilly and Company, Indianapolis, IN
- ThP 538 **Disulfide Bond Mapping-A Case Study through Partial Reduction;** Song Klapoetke; KBI, Durham, NC
- ThP 539 **Innovator and Biosimilar Infliximab: Comparability Assessment of the Host Cell Proteins and Protein Higher Order Structure;** Jing Fang¹; Catalin E Doneanu¹; William R Alley¹; Ying-Qing Yu¹; Asish Chakraborty¹; Alain Beck²; Weibin Chen¹; ¹Waters, Milford, MA; ²Centre d'Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France
- ThP 540 **Protein Conformational Analysis of Native and Stressed Monoclonal Antibodies using Ion Mobility and LC/MS/MS Disulfide Bond Mapping;** David L Wong¹; Stephen O Gregory¹; Jordy Hsiao¹; Te-Wei Chu¹; Stephen Madden¹; Javier Satulovsky¹; ¹Agilent Technologies, Santa Clara, CA
- ThP 541 **Mapping of Disulfide Bonds by Reducing Electrochemistry and Mass Spectrometry;** Christian Cramer¹; Kim F. Haselmann¹; Jesper V. Olsen²; Peter Kresten Nielsen¹; ¹Novo Nordisk A/S, Måløv, Denmark; ²NNF Center for Protein Research, University of Copenhagen, Denmark
- ThP 542 **Protein Dynamics in the TGF- β Superfamily by Hydrogen Deuterium Exchange Mass Spectrometry;** Roxana E. Iacob¹; Viet Le²; Bo Zhao²; Yuan Tian²; Timothy A. Springer²; John R. Engen³; ¹Northeastern University, Boston, MA; ²Children's Hospital Boston and Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA; ³Northeastern University, Boston, MA
- ThP 543 **Characterizing Deamidation and Oxidation in Adalimumab with Low pH Peptide Mapping and Middle-Up Mass Spec Analysis;** Chris Hosfield¹; Eric Largy²; Anicet Catrain²; Fabrice Cantais²; Gery Van Vyncht²; Michael M Rosenblatt¹; Sergei Savelyev¹; Marjeta Urh¹; Arnaud Delobel²; ¹Promega Corporation, Madison, WI; ²Quality Assistance, Thuin, Belgium
- ThP 544 **Deciphering Biotherapeutic Protein Disulfide Bonds by Top and Middle-Down Mass Spectrometry;** Jiang Zhang¹; Pilsoo Kang¹; Jianmei Kochling¹; ¹Sanofi Genzyme, Framingham, MA
- ThP 545 **Investigation of Antibody Aggregates by Hydrogen / Deuterium Exchange Mass Spectrometry and Other Biophysical Tools;** Richard Yu-Cheng Huang¹; Deqiang Yu²; Yuanli Song²; Ryan K. Swanson²; Zhijun Tan²; Elizabeth Schutsky²; Angela Lewandowski²; Zhengjian Li²; Guodong Chen¹; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Devens, MA
- ThP 546 **Disulfide Bond Identification of Biotherapeutic Proteins using Various Fragmentation Techniques Available on an Orbitrap Fusion Tribrid Mass Spectrometer;** Stephane Houel¹; Jennifer Sutton¹; Seema Sharma¹; Terry Zhang¹; Romain Huguet¹; Martin Samonig²; Vlad Zabrouskov¹; Jonathan Josephs¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Germering, Germany
- ThP 547 **Rapid Profiling of Stressed PEGylated Protein Pharmaceuticals using Ion-Exchange Chromatography with Online Detection by Native ESI and Top-Down MS/MS;** Khaja Muneeruddin¹; Cedric E Bobst¹; Ruth Frenkel²; Damian Houde²; Iva Turyan²; Zoran Susic²; Igor A Kaltashov¹; ¹University of Massachusetts, Amherst, MA; ²Biogen, Cambridge, MA
- ThP 548 **A High-Throughput, Automated Platform Method for Multi-Attribute LC-MS Analysis of Cell Culture Harvest and Antibody Glycosylation;** Jia Dong¹; Nicole Migliore¹; Steven J Mehrman¹; John Cunningham¹; Michael J Lewis¹; Ping Hu¹; ¹Janssen Research & Development, Malvern, PA
- ThP 549 **Automated Data Analysis Enabling Mass Spectrometry-based Assays for the Developability Assessment of Biotherapeutics;** Maurizio Bronzetti¹; Cassandra Wigmore²; Joe Shambaugh¹; David Bush¹; Arnd Brandenburg²; Peter Haberl³; ¹Genedata Inc, Lexington, MA; ²Genedata AG, Basel, Switzerland; ³Genedata GmbH, Munich, Germany
- ThP 550 **Characterization of Selected Therapeutic Monoclonal Antibodies under Stressed Conditions;** Robert Carney¹; Zsuzsa Lakos¹; Elena Dremina¹; John Snyder¹; ¹Eurofins Lancaster Laboratories, Inc., Lancaster, PA
- ThP 551 **Site-specific Glycoform Mapping of Biotherapeutics with Micro-Heterogeneity and Macro-Heterogeneity;** Yongsuk Seo^{1,2}; Myung Jin Oh^{1,2}; David Bradley³; Hyun Joo An^{1,2}; ¹AGRS, Chungnam National University, Daejeon, Korea; ²GRAST, Chungnam National University, Daejeon, Korea; ³Agilent Technologies, Santa Clara, CA
- ThP 552 **Biosimilar Insulin Characterization: Top/Middle/Bottoms up Approaches;** Rishikant Gupta¹; Mithun Bhatt¹; Annu Uppal²; Manoj Pillai²; Archana Krishnan¹; Sanjay Sonar¹; ¹Biogenomics, Thane (w), Mumbai, India; ²SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India
- ThP 553 **Mass Spectrometry Based Comparison of Rituximab Originator and Biosimilar;** Othman Montacir¹; Murat Eravci²; Andreas Springer³; Stephan Hinderlich⁴; Maria Kristina Parr¹; ¹Institute of Pharmaceutical and Medicinal Chemistry, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; ²Institut für Chemie und Biochemie, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; ³Großgerätezentrum BioSupraMol, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; ⁴Beuth Hochschule für Technik Berlin - University of Applied Sciences, Department of Life Sciences and Technology, Berlin, Germany, Berlin, Germany
- ThP 554 **Towards the Fast and Increasingly Simplified Analysis of Trisulfide Formation in Biopharmaceutical Antibodies;** Anja Resemann¹; Rainer Paape¹; Christoph Nordmann¹; Waltraud Evers¹; Lars Vorwerk¹; Eckhard Belau¹; Volker Sauerland¹; Lisa A Marzilli²; Jason C Rouse²; Jason S Wood³; Detlev Suckau¹; ¹Bruker Daltonic GmbH, Bremen, Germany; ²Biotherapeutics Pharm. Sci., Pfizer Inc. Andover, MO; ³Bruker Daltonic, Billerica, MA
- ThP 555 **Site-Specific Characterization and Quantitation of Protein Pegylation by LC-UV-MS and Standard Addition Approach;** Yanjun Liu¹; Shiao-Lin Wu^{1,2}; William Hancock¹; ¹Barnett Inst., Northeastern University Boston, MA; ²BioAnalytix Inc, Cambridge, MA
- ThP 556 **High Resolution Separations for Protein LC/MS;** Barry Boyes¹; Benjamin Libert²; Stephanie E Schuster²; Brian E Wagner²; William E Miles²; Joseph Kirkland²; ¹Advanced Materials Technology Inc, Wilmington, DE; ²Advanced Materials Technology Inc, Wilmington, DE
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- Scheffler²; Stephane Houel¹; Jonathan L Josephs¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, DE
- ThP 558 **Characterization of Therapeutic Protein Charge Heterogeneity by Isoelectric Focusing and Nano-spray LC-MS**; Janet Lau¹; Chen Li¹; Shiao-Lin (Billy) Wu¹; ¹BioAnalytix Inc, Cambridge, MA
- ThP 559 **Separation and Characterization of IgG2 Disulfide Isoforms by pH Gradient Cation Exchange Chromatography and Non-Reduced LC/MS - Peptide Mapping**; Kristin J Boggio¹; Anastasiya P Manuilov¹; Thomas J Porter¹; Jason C Rouse¹; Tanya Q. Shang¹; Matthew C Thompson¹; ¹Pfizer Inc, Andover, MA
- ThP 560 **High Throughput Screening and Characterization of Bispecifics Using Native Ion Mobility Mass Spectrometry**; Caroline S. Chu¹; Te-Wei Chu¹; Gregory O Staples¹; Patrick D Perkins¹; Andy Gieschen²; Christian Klein¹; Carol H. Ball³; Ning Tang¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, La Jolla, CA; ³Agilent Technologies, Wilmington, DE
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- ThP 564 **On-line Disulfide Cleavage for Structural Characterization**; J.C. Yves Leblanc¹; Tanya Gamble²; ¹SCIEX, Concord, ON; ²SCIEX, Concord ON, Canada
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- ThP 566 **An Investigation into A β /Metal Binding via MALDI TOF MS**; Andrea Renee Kelley¹; George Perry¹; Stephan B.H. Bach¹; ¹University of Texas at San Antonio, San Antonio, TX
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- ²Department of Pathology, University of Michigan, Ann Arbor, MI; ³Department of Chemistry, University of Michigan, Ann Arbor, MI; ⁴Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI
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- ThP 575 **Structural Characterization of a G Protein-GEF Complex Using Top-Down Ultraviolet Photodissociation Mass Spectrometry**; W. Ryan Parker¹; Matthew Montana Quick²; Elisa Novelli²; Lauren Webb²; Jennifer S Brodbelt²; ¹University of Texas at Austin, Austin, TX; ²University of Texas, Austin, Austin, TX
- ThP 576 **Structural Characterization of Myokine-Ligand Complexes Using Top-Down Ultraviolet Photodissociation Mass Spectrometry**; Rachel Mehaffey¹; Michael Cammarata¹; Jennifer S Brodbelt¹; ¹The University of Texas, Austin, Texas
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- ThP 579 **Mechanism of Prion Oligomerization as Determined by Structural Proteomics**; Jason J Serpa¹; Evgeniy V Petrochenko¹; Christoph H. Borchers^{1,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
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- ThP 581 **Identification of Hidden Allosteric Sites of β -Lactamase by Dynamic Simulation and Mass Spectrometry;** Supratik Dutta¹; Sukrit Singh²; Gregory R Bowman³; Michael L Gross³; ¹Washington University in St. Louis, Chesterfield, Missouri; ²Washington University in St. Louis, St. Louis, MO; ³Washington University in St. Louis, Saint Louis, MO
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- ThP 585 **Higher-Throughput Native Mass Spectrometry for Protein-Ligand Screening with Application for Trimethoprim-Resistant Dihydrofolate Reductase;** Michael Cammarata¹; Ross Thyer¹; Andrew Ellington¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
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- ThP 588 **N-glycoproteome Profiling of the Mouse Testis;** Xuejiang Guo¹; Fangjuan Liu¹; Yueshuai Guo¹; Tao Zhou¹; Zhou Zuomin¹; Jiahao Sha¹; ¹Nanjing Medical University, Nanjing, CN
- ThP 589 **Sample Displacement Chromatography (SDC) for Differentiating Glycoforms on Human Glycoproteins for Cancer Biomarker Discovery;** Wonryeon Cho¹; Jihoon Shin¹; ¹Wonkwang University, IKSAN, Jeonbuk
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- ThP 591 **Comparative Analysis of Histone PTMs using DDA, DIA and PRM Methods on a QExactive HF Orbitrap;** Joby Cole¹; Eleanor Hanson²; David Dockrell^{3,4,5}; Mark Dickman^{2,5}; ¹University of Sheffield, Sheffield, South Yorkshire; ²Department of Chemical and Biological Engineering,
- University of Sheffield, Sheffield, UK; ³Department of Infection, Immunity and Cardiovascular Sciences, University of Sheffield Medical School, Sheffield, UK; ⁴Sheffield Teaching Hospitals NHS FT, Sheffield, UK; ⁵The Florey Institute, University of Sheffield, Sheffield, UK
- ThP 592 **Altered Lysine Acylation of Mitochondrial Proteins in Response to Macronutrient Stresses in the Mouse Liver;** Jesse G. Meyer¹; Natan Basisty¹; Samir Softic²; Birgit Schilling¹; Kahn C. Ronald²; Bradford W Gibson¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Joslin Diabetes Center and Harvard Medical School, Boston, MA
- ThP 593 **Proteome wide Profiling of Protein Lysine Propionylation in *Escherichia coli*;** Mingwei Sun¹; Linhui Zhai¹; Yingming Zhao^{1,2}; Minjia Tan¹; ¹Shanghai Institute of Materia Medica, Shanghai, P. R. China; ²The University of Chicago, Chicago, IL
- ThP 594 **A Ubiquitin-Conjugating Enzyme Mediates Global Remodeling of the Proteome during Terminal Differentiation;** Miguel Prado¹; Anthony Tuan Nguyen¹; Mingwei Min¹; Joao A Paulo¹; Yuan Shi¹; Mona Kawan¹; Verena Dederer¹; Paul Schmidt²; Dean Campagna²; Mark D Fleming²; Steven P Gygi¹; Daniel Finley¹; ¹Harvard Medical School, Boston, MA; ²Boston Children's Hospital, Harvard Medical School Boston, MA
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- ThP 600 **Identification and Characterization of Hydroxylysines in an Immunoglobulin;** Verena Niggeloh¹; Georg Drabner¹; ¹Roche Innovation Center Penzberg, Penzberg, Germany
- ThP 601 **Dynamic Remodeling of Protein Acetylation in *E. coli* in Response to Different Carbon Sources;** Birgit Schilling¹; David Christensen²; Jesse G Meyer¹; Alexandria K D'Souza¹; Dylan J Sorensen¹; Nicholas Shulman³; Brendan MacLean³; Christopher V Rao⁴; Alan J Wolfe²; Bradford W Gibson¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Loyola University Chicago, Maywood, IL; ³University of Washington, Seattle, WA; ⁴University of Illinois at Urbana-Champaign, Urbana, IL
- ThP 602 **Identification of Prenylome by Chemical Oxidation and CID and ETD Tandem Mass Spectrometry;** Ada Shahinuzzaman¹; Ruchika Bhawal¹; Saiful Chowdhury²; ¹University of Texas at Arlington, Arlington, TX; ²University of Texas at Arlington, Arlington, TX
- ThP 603 **Proteomics Analysis of Toxoplasma gondii Palmitoylated Proteins and its Impact on Rhoptry Localization;** Bin Deng¹; Marina C Caballero²; Andrés M

- Alonso²; Marcia Attias³; Wanderley de Souza³; Maria M Corvi²; ¹University of Vermont, Burlington, VT; ²Laboratorio de Parasitologia Molecular, Instituto de Investigaciones Biotecnológicas-Instituto Tecnológico de Chascomús (IIB-INTECH), Universidad Nacional de San Martín (UNSAM) - Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Chascomús, Argentina; ³Laboratório de Ultraestrutura Celular Hertha Meyer, Instituto de Biofísica, Carlos Chagas Filho and Instituto Nacional de Ciência e Tecnologia em Biologia Estrutural e Bioimagens Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
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- ThP 615 **Reverse Phased Dispersive Micropipette Tip Extraction with Multiple Fractionation Strategy for Proteomic Profiling of Human Biofluids for Potential Clinical Applications**; Yuzhe Nie¹; Qian Wang¹; Mullis Todd²; William Brewer¹; L. Andrew Lee³; ¹University of South Carolina, Columbia, SC; ²IMCS, LLC, Columbia, SC; ³IMCS, Columbia, South Carolina
- ThP 616 **Profiling Protein Expression in Limited Amount of Mouse Cortex using CE-ESI-HRMS**; Eric Corcoran¹; Peter Nemes²; Marta Zamarbide²; Chiara M. Manzini²; ¹George Washington University, Washington, DC; ²The George Washington University, Washington, DC
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- ThP 624 **Investigation of the Crosstalk between Phosphorylation and Cysteine Modifications using a Novel Cysteine Tag in Combination with TiO2 Chromatography**; Honggang Huang¹; Giuseppe Palmisano²; Martin R Larsen³; ¹University of Southern Denmark, Odense M, Denmark; ²Department of Parasitology, ICB, University of São Paulo,

São Paulo, BRASIL; ³Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense M, Denmark

- ThP 625 **Methodology to Fish Peptide Ligands of nAChRs from Cone Snail Venoms by MALDI-TOF Mass Spectrometry;** Julien Echterbille¹; Nicolas Gilles²; Romulo Araoz²; Edwin De Pauw¹; Loïc Quinton¹; ¹Laboratory of Mass Spectrometry - University of Liege, Liege, Belgium; ²Commissariat à l'Energie Atomique - DSV/SIMOPRO- Toxins, Receptors and Channels team, Saclay, France

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- ThP 628 **Use of QconCAT Quantitation Data to Resolve 'Hubs' in the Protein Crosslinkome of a Relatively Rigid-Body Protein Complex;** Ji-Suk Kim¹; Robert Beynon²; Paul Gershon¹; ¹UC-Irvine, Irvine, CA; ²University of Liverpool, Liverpool, UK
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- ThP 635 **Quantitative Analysis of AKT/mTOR Pathway using Multiplex-Immunoprecipitation and Targeted Mass Spectrometry;** Bhavin Patel¹; Alex Behling¹; Leigh Foster¹; Shouling Xu²; Ryan Bomgarden¹; Carrie Clothier¹; Kay Opperman¹; Rosa I Viner²; Andreas Huhmer²; John C Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA
- ThP 636 **Application of Stochastic Protein Turnover Model to *in vivo* and *in vitro* Studies;** Mahbubur Rahman¹; Rovshan Sadygov¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX
- ThP 637 **Direct Measurement and Modeling of Protein Synthesis and Degradation Dynamics during Chemotherapeutic Response in Multiple Myeloma;** Tzu-Yu Liu^{1,2}; Hector Han-Li Huang³; Diamond D Wheeler³; Yun S Song^{1,2}; Arun Paul Wiita³; ¹UC Berkeley, Berkeley, California; ²University of Pennsylvania, Philadelphia, PA; ³UCSF, San Francisco, CA
- ThP 638 **Effects of Cigarette Smoke, Cessation and Switching to Two Heat-Not-Burn Tobacco Products on Lung Lipid Metabolism Intwo Mouse Strains;** Thomas Schneider¹; Bjoern Titz¹; Stephanie Boue¹; Blaine Phillips²; Terhi Vihervaara³; Marja Talikka¹; Catherine Nury¹; Ashraf Elamin¹; Florian Martin¹; Walter Schlage¹; Nikolai V. Ivanov¹; Patrick Vanscheeuwijck¹; Manuel C. Peitsch¹; Julia Hoeng¹; ¹Philip Morris International, Neuchatel, Switzerland; ²Philip Morris International Research Laboratories, Singapore, Singapore; ³Zora Biosciences Oy, Biologinkuja, Finland
- ThP 639 **Differential Protein Expression Analysis by Mass Spectrometry as a Service;** Claudia Fortes¹; Jonas Grossmann¹; Paolo Nanni¹; Witold Wolski¹; Christian Panse¹; Laura Kunz¹; Christian Trachsel¹; Nathalie Selevsek¹; Can Türker¹; Ugur Gürel¹; Bernd Roschitzki¹; Ralph Schlapbach¹; ¹Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland
- ThP 640 **Targeted Proteomics Coming of Age: SRM, PRM and DIA Performance Evaluated from a Core Facility Perspective;** Paolo Nanni¹; Tobias Kockmann¹; Christian Panse¹; Christian Trachsel¹; Jonas Grossmann¹; Witold Wolski¹; Nathalie Selevsek¹; Asa Wahlander¹; Ralph Schlapbach¹; ¹FGCZ, Univ Zurich Zurich, Switzerland
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- ThP 642 **Neutron-encoded Protein Quantification Integrated in the MaxQuant Platform Allows Highly Accurate and Multiplexed Quantification;** Anna E Merrill¹; Katherine Overmyer¹; Derek J Bailey¹; Nicholas W Kwiecien¹; Alex S Hebert¹; Michael S Westphall¹; Stefka Tyanova²; Joshua J Coon¹; Juergen Cox²; ¹University of Wisconsin Madison, Madison, WI; ²Max-Planck-Institute of Biochemistry, Martinsried, Germany
- ThP 643 **Development of Universal MS Signal Processor for Improved Data Independent Acquisition Performance;** Yet-Ran Chen; Academia Sinica, Taipei, Nankang
- ThP 644 **Extreme Discordance in Kinase Quantification Using Isobaric Labeling and Parallel Reaction Monitoring with Stable Isotope Dilution Mass Spectrometry;** Robert William Sprung, Jr.¹; Qiang Zhang¹; Petra Erdmann-Gilmore¹; Sherri R Davies¹; Rose Connors¹; Yiling Mi¹; Gary Johnson²; Matthew R Meyer¹; Shunqiang Li¹; R. Reid Townsend¹; ¹Department of Medicine, Washington University School of Medicine, Saint Louis, MO; ²Department of Pharmacology, University of North Carolina School of Medicine, Chapel Hill, NC

- ThP 645 **Integrating Protease-Specific Micorarrays (CLIP-CHIP) with Proteomics (SILAC) and Terminomics (TAILS) to Profile Macrophage Differentiation;** Nestor Solis¹; Antoine Dufour¹; Reinhild Kappelhoff¹; Anders Kristensen²; Leonard Foster¹; Christopher M Overall¹; ¹University of British Columbia, Vancouver, Canada; ²BC Cancer Agency, Vancouver, Canada
- ThP 646 **2H-metabolic Labeling Approach Reveals Reduced Synthesis of Hepatic Mitochondrial Proteins in a Mouse Model of NASH;** Kwangwon Lee¹; Abdullah Osme¹; Ling Li²; Zhicheng Jin¹; Belinda Willard²; Rovshan Sadygov³; Takhar Kasumov¹; ¹Northeast Ohio Medical University, Rootstown, OH; ²Cleveland Clinic Lerner Research Institute, Cleveland, OH; ³University of Texas Medical Branch at Galveston, Galveston, TX
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- ThP 651 **Diagnosis of Thymoma Subtypes Using Proteomic Signatures Detected by Mass Spectrometry;** Linan Wang¹; Owen Branson¹; Konstantin Shilo¹; Charles Hitchcock¹; Michael A. Freitas¹; ¹Ohio State University, Columbus, OH
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- ThP 653 **Deep Proteome Analysis of Murine Islets;** Elyse Freiburger¹; Mark Keller¹; Alexander S Hebert¹; Donald S Stapleton¹; Alan D Attie¹; Joshua J Coon¹; ¹UW-Madison, Madison, WI
- ThP 654 **Rapid Proteomic Profiling of Human Plasma;** Gary M. Wilson¹; Evgenia Shishkova¹; Alex S Hebert¹; Michael S Westphall¹; Joshua J Coon¹; ¹UW-Madison, Madison, WI
- ThP 655 **Protein Turnover Rate in Mice Gastrointestinal Tract is Affected by the Spatial Location and The Microbiota;** Liisa Arike¹; Andrus Seiman²; Sjoerd van der Post¹; Ana Maria Rodriguez Piñero¹; Anna Ermund¹; André Schütte¹; Malin E. V. Johansson¹; Fredrik Bäckhed³; Gunnar C Hansson¹; ¹Department of Medical Biochemistry, University of Gothenburg, Gothenburg, Sweden; ²Competence Centre of Food and Fermentation Technologies, Tallinn, Estonia; ³Department of Molecular and Clinical Medicine, Wallenberg Laboratory, University of Gothenburg, Gothenburg, Sweden
- ThP 656 **A Brain Regional Proteomic Atlas in Mouse;** Jong Min Choi¹; Sung Yun Jung¹; Maxime William C. Rousseaux¹; Anna Malovannaya¹; Jin Jieun Kim¹; Joachim Kutzera²; Yi Wang¹; Yin Huang³; Weimin Zhu³; Suman Maity¹; Huda Yahya Zoghbi¹; Jun Qin¹; ¹Baylor College of Medicine, Houston, TX; ²University of Amsterdam, Amsterdam, The Netherlands; ³Beijing Proteome Research Center, Beijing, China
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- ThP 658 **Proteomics and Imaging Mass Spectrometry of High-Grade Serous Ovarian Cancer Reveals Marked Intratumoral Alterations in Neoadjuvant Chemotherapy-Treated Patients;** Emily R Penick^{1,2}; Nicholas W Bateman^{2,3}; Jessica Moore⁴; Brian L Hood²; Jeremy L Norris⁴; David Cohn⁵; Laura Havrilesky⁶; Andrew Berchuck⁶; Chad Hamilton^{1,2,3}; George Maxwell^{2,3,7}; Richard M Caprioli⁴; Thomas P Conrads^{2,3,8}; ¹Walter Reed National Military Medical Center, Department of Obstetrics and Gynecology, Bethesda, MD; ²Women's Health Integrated Research Center, Annandale, VA; ³John P. Murtha Cancer Center, Bethesda, MD; ⁴Vanderbilt University School of Medicine, Nashville, TN; ⁵Ohio State University, Columbus, OH; ⁶Duke University Medical Center, Durham, NC; ⁷Inova Fairfax Hospital, Department of Obstetrics & Gynecology, Falls Church, VA; ⁸Inova Schar Cancer Institute, Falls Church, VA
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- ThP 664 **Label-Free Quantitative Differential Expression Proteomics of Formalin-Fixed Paraffin-Embedded Liver Biopsy Samples from a Longitudinal Study of Hepatitis C Patients;** Sarah Mabbett¹; Will J Thompson¹; Joseph Lucas¹; Keyur Patel²; Arthur Moseley¹; ¹Duke University Medical Center, Durham, NC; ²University of Toronto, Toronto ON, Canada
- ThP 665 **Proteomic Mapping of Enamel Matrix in Mice with Different Susceptibilities to Dental Fluorosis by Gel-Based and Gel-Free Approaches;** Aline Leite¹; Mileni Silva Fernandes²; Senda Charone²; Gary M Whitford³; Eric T Everett⁴; Marília Afonso Rabelo Buzalaf²; ¹University of São Paulo, São Paulo, SP; ²University of São Paulo, Bauru, SP-Brazil; ³University of Georgia, Atlanta, GA; ⁴University of North Carolina, Chapel Hill, NC
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- ThP 673 **Nitrite-Induced Preconditioning Elicits Significant Long-Term Alterations to Key Heart Proteins Involved in Redox Stress Protection and Mitochondrial Function;** David H. Perlman^{1,1}; Giuseppe Infusini¹; Selena Bauer¹; Bernadette O Fernandez¹; Mark E McComb¹; Martin Feilisch¹; Catherine E Costello¹; ¹Boston University School of Medicine, Boston, MA
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- ³Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan (R.O.C.)
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- ThP 682 **High Throughput Quantitation for Therapeutic Drug Monitoring with Open Access LC/MS/MS System;** Miho Kawashima¹; Yoshihiro Hayakawa²; Taku Tsukamoto²; Masafumi Kikuchi³; Masaki Tanaka³; Shinya Takasaki³; Hiroaki Yamaguchi³; Nariyasu Mano³; ¹Shimadzu Corporation, Tokyo, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Tohoku University Hospital, Sendai, Japan
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- ThP 698 **Highly Sensitive and Selective Bioanalytical Quantitation Method for Docetaxelin Human Plasma;** santosh kapil kumar Gorti¹; Aman Sharma¹; Jeyan Albert¹; Anoop Kumar¹; Manoj Pillai¹; ¹SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India

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- ThP 700 **Defining the Consequences of Genetic Variation on a Proteome- and Phosphoproteome-Wide Scale;** Joel Chick¹; Steven C Munger²; Petr Simecek²; Edward L Huttlin¹; Kwangbom Choi²; Dan Gatti²; Narayanan Raghupathy²; Karen Svenson²; Gary Churchill²; Steven P

Gygi¹; ¹Harvard Medical School, Boston, MA; ²The Jackson Laboratory, Bar Harbor, ME

- ThP 701 **Selectivity Profiling of Kinase Inhibitors - From Label Free DDA Quantification to Spectral Libraries for Sub-Proteomes;** Susan Klaeger^{1,2,3}; Stephanie Heinzlmeir^{2,3,4}; Mathias Wilhelm¹; Maria Reinecke¹; Dominic Helm¹; Huichao Qiao¹; Guillaume Médard¹; Bernhard Kuster^{1,5}; ¹Technical University Munich, Munich; ²German Cancer Consortium (DKTK), Munich, Germany; ³German Cancer Research Center, Heidelberg, Germany; ⁴Freising; ⁵Center for Integrated Protein Science, Munich, Germany
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- ThP 703 **Proteome Wide Selectivity Profiling of Cyclin-dependent Kinase Inhibitors;** Huichao Qiao¹; Susan Klaeger^{1,2,3}; Mathias Wilhelm¹; Stephanie Heinzlmeir^{1,2,3}; Dominic Helm¹; Guillaume Médard¹; Bernhard Kuster^{1,4}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²German Cancer Consortium (DKTK), Munich, Germany; ³German Cancer Research Center, Heidelberg, Germany; ⁴Center for Integrated Protein Science, Munich, Germany
- ThP 704 **A Comprehensive Study of the Ponatinib-Induced Kinome Changes in Drug-Resistant Leukemia;** Laura Herring¹; Denis Okumu¹; Karim Gilbert¹; Michael East¹; Lee Graves¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
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- ThP 708 **PKCε and CDKs Regulate Insulin Signaling in Response to a 3-Day High Fat Diet;** Brandon Gassaway^{1,2}; Max Petersen^{1,3}; Hans Rudolf Aerni^{1,2}; Yulia Surovtseva⁴; Karl W Barber^{1,2}; Joshua B Sheetz¹; Svetlana Rogulina¹; Janie Merkel⁴; Varman Samuel^{1,5}; Gerald Shulman^{1,3}; Jesse Rinehart^{1,6}; ¹Yale School of Medicine, New Haven, CT; ²Systems Biology Institute, West Haven, CT; ³Howard Hughes Medical Institute, Chevy Chase, MD; ⁴Yale Center for Molecular Discovery, West Haven, CT; ⁵Veterans Affairs

- Medical Center, West Haven, CT; ⁶Systems Biology Institute, Yale University, West Haven, CT
- ThP 709 **Profiling Changes in the Phosphoproteome of Hematopoietic Cells in Response to a Novel Class of Anti-Oncogenic Sphingolipid Derived Small Molecules;** Peter Kubiniok¹; Alison McCracken²; Michael Perryman¹; Stephen Hanessian¹; Aimee Edinger²; Pierre Thibault¹; ¹University of Montreal, Montreal Qc, Canada; ²University of California - Irvine, Irvine, CA
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