



Welcome to the 65th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Indiana Convention Center. Corporate Member hospitality suites are located in the JW Marriott Hotel.

SPONSORS

ASMS gratefully acknowledges the support of these companies.



CONTRIBUTOR

Advanced Energy

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GENERAL INFORMATION

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

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

4:00 - 4:45 pm, Sunday, Room 107-110, level 1

Plan Your Strategy: What to See and Do at ASMS

TUTORIALS

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

Hall D, level 1



5:00 - 5:45 pm

MALDI: Past and Future

Kermit K. Murray

Louisiana State University



5:45 - 6:30 pm

Cancer Immunotherapy and Mass Spectrometry

Donald F. Hunt

University of Virginia

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

Wabash, level 1



5:00 - 5:45 pm

Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life

Erin S. Baker

Pacific Northwest National Laboratory



5:45 - 6:30 pm

CE/MS - Ready for Prime Time?

Norman J. Dovichi

University of Notre Dame

PLENARY SESSIONS

SUNDAY PLENARY SESSION, 6:45 - 7:45 PM

Hall D, level 1



Welcome

Richard A. Yost

University of Florida

ASMS Vice President for Programs



Towards a Good Start in Life: Neonatal Screening and Beyond

David S. Millington

Duke University Medical Center

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

Poster/Exhibit Hall. Conference name badge is required.

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

Hall D, level 1



Award for a Distinguished Contribution in Mass Spectrometry

Catherine E. Costello

Boston University

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

Hall D, level 1



Biemann Medal

Ryan Julian

University of California, Riverside

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

Hall D, level 1



Saving the Great Coral Reefs

Kristen Marhaver

Research Station Carmabi

THURSDAY CLOSING EVENT AT THE INDIANA STATE MUSEUM, 6:30-9:00 PM, \$30/PERSON

Tickets must be purchased in advance by Monday 12 noon.



GENERAL INFORMATION



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 D

Session B (MOB, TOB, WOB, ThOB) 500 Ballroom

Level 2

Session C (MOC, TOC, WOC, ThOC) Sagamore 1-3

Session D (MOD, TOD, WOD, ThOD) Sagamore 4

Session E (MOE, TOE, WOE, ThOE) Sagamore 5-7

Level 1

Session F (MOF, TOF, WOF, ThOF) Wabash

Session G (MOG, TOG, WOG, ThOG) Room 101-106

Session H (MOH, TOH, WOH, ThOH) Room 107-110

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 ready room is 117, level 1. 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 Welcome Reception 7:45 pm - 9:00 pm

Monday - Wednesday 7:30 am - 8:00 pm

Thursday 7:30 am - 2:30 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 Reception 7:45 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 AND INTERNET STATIONS are available 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 slides will be printed to PDF and used as proceedings submission for speakers who fail to submit on their own.**

WEBCASTING includes tutorial lectures, plenary lectures, and oral sessions. Webcasts will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in webcasts.

CORPORATE HOSPITALITY SUITES may be open 8:00 - 10:30 pm, Monday through Wednesday. Suites are located in the **JW Marriott 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.

Sunday 7:45 - 9:00 pm

Monday - Wednesday 7:30 am - 5:00 pm

Thursday 7:30 am - 2:30 pm

GUEST REGISTRATION (\$10) includes designated name badge and entrance to the Sunday evening welcome 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 208, level 2 (for mothers-only).



GENERAL INFORMATION

TWO IMPORTANT OPPORTUNITIES IN THE POSTER/EXHIBIT HALL

1. **INFORMATICS HUB**
Meet up with experts to discuss your informatics questions.
2. **FUNDING AGENCY "OFFICE HOURS"**
Consult with program officers and representatives from the major U.S. funding agencies.

VISIT THE JASMS BOOTH NUMBER 111

1. Meet the Editor
2. Learn about submitting your ASMS presentation for publication

CONFERENCE REGULATIONS

Please review these policies which are intended to assure the comfort and privacy of all conference participants.

Name badge is required for all conference sessions, including the Poster/Exhibit Hall and Career Center, and off site events such as the hospitality suites and closing event (ticket required).

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
JW Marriott	(317) 860-5800
Marriott Downtown	(317) 822-3500
Westin	(317) 262-8100
Hyatt Regency	(317) 632-1234
Omni Severin	(317) 634-6664
Crowne Plaza	(317) 631-2221

Hotel	Telephone
Hampton Inn & Suites	(317) 856-1000
Courtyard by Marriott	(317) 822-9029
Fairfield Inn & Suites (downtown)	(317) 636-7678
Springhill Inn (downtown)	(317) 972-7293
Hilton Garden Inn (downtown)	(317) 955-9700
Homewood Suites (downtown)	(317) 636-7992





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CONGRATULATIONS

to these members who were elected to the ASMS Board

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Cambridge, MA

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Notre Dame, IN

STAFF

Judith A. Sjoberg, *Executive Director*
Jennifer Watson
Lola Priest, Miquela Sena
Marin Walker, Brent Watson



INTEREST GROUP COORDINATORS

<i>Analytical Laboratory Managers</i>	Emily Chen Aliss Chien
<i>Bioinformatics for MS</i>	Meena Choi Samuel Payne
<i>Biotherapeutics</i>	Charles Cheng Ashley Gucinski Ruth
<i>Clinical Chemistry</i>	Tim Garrett
<i>Data Independent Acquisition</i>	Ben Collins Ludovic Gillet
<i>Drug Metabolism & Pharmacokinetics</i>	Mark Cancilla Philip Tiller
<i>Energy, Petroleum & Biofuels</i>	Mark Barrow David Stranz
<i>Environmental Applications</i>	Marc Engel Achille Cappiello
<i>Exposomics</i>	H. M. Skip Kingston Anthony Macherone
<i>Flavor, Fragrance and Foodstuff</i>	Sara Kern David Schroeder
<i>Forensics & Homeland Security</i>	Kenyon Evans-Nguyen Adam Hall
<i>FTMS</i>	Melinda McFarland David Kilgour
<i>Fundamentals</i>	Victor Ryzhov Michael Van Stipdonk
<i>H/D Exchange, Covalent Labeling & Cross Linking</i>	Lan Huang David Weis
<i>Imaging MS</i>	Reid Groseclose Raf Van de Plas
<i>Ion Mobility MS</i>	Valerie Gabelica Stephen Valentine
<i>Ion Trap MS</i>	Zheng Ouyang Wei Xu
<i>Lipids & Lipodomics</i>	Eva Duchoslav Todd Mitchell
<i>LC/MS Related Topics</i>	Eric Soderblom Will Thompson
<i>Metabolomics</i>	John Bowden Tim Garrett
<i>Metal Ion Coordination Chemistry</i>	Eric Dodds Cheng Lin
<i>Oligonucleotides & Nucleic Acids</i>	Patrick Limbach Laixin Wang
<i>Pharmaceuticals</i>	Matthew Schenauer John Valliere-Douglass
<i>Photoionization MS</i>	Eleanor Riches Ralf Zimmerman
<i>Polymeric Materials</i>	Christina Mastromatteo Stephen Rumbelow
<i>Regulated Bioanalysis</i>	Fabio Garofolo Jian Wang

INTEREST GROUP COORDINATORS (CONTINUED)

<i>Undergraduate Research in MS</i>	Megan Gessel James Pesavento
<i>Young Mass Spectrometrists</i>	Violet Lee Doug Phanstiel

COMMITTEES

<i>Asilomar Conference (ACMS)</i>	Matt Bush Benjamin Garcia Lingjun Li Jenny Brodbelt (ASMS Board Rep.)
<i>Corporate Liaison</i>	Jack Henion, Chair Jenny Brodbelt (ASMS Board Rep.) Martin Eysberg, Antec Carol Harp, Agilent Maureen Quaranta, Shimadzu Bobbie Jo Seyler, MilliporeSigma Paul Speir, Bruker Annik Stolk, Canadian Life Science
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<i>Publications</i>	Facundo Fernandez, Chair Lorna De Leoz Valerie Gabelica Jody C. May Will Thompson Joseph Loo (ex officio)
<i>Sanibel Conference</i>	Melinda McFarland Fanyu Meng Victor Ryzhov Ying Ge (ASMS Board Rep.)

AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2017 RECIPIENT: CATHERINE E. COSTELLO

AWARD LECTURE: 4:45 PM, MONDAY, HALL D, LEVEL 1



Dr. Catherine E. Costello is the recipient of the 2017 Award for a Distinguished Contribution in Mass Spectrometry for her pioneering contributions to the development of tandem mass spectrometry of glycans and glycoconjugates.

Glycans differ from proteins in that their biosynthesis derives from a series of enzymatic reactions in the endoplasmic reticulum and Golgi apparatus and not from a template-driven process. Glycans, depending on class, may be branched, meaning that their structural determination requires determination of linkage positions and stereochemistry. The function of a glycan depends on the target to which it binds. A difference in a single monosaccharide linkage in a glycan alters the partners to which a glycan or glycoconjugate binds. For glycoproteins, the large number of proteoforms reflect glycan heterogeneity at each glycosylation site. Thus, the population of glycoprotein proteoforms present at any given place

or time differ in their capacities to bind to partners that contain carbohydrate binding domains. The complexity of glycan and glycoconjugate structures presents a severe analytical challenge to the field of glycomics.

Prof. Costello's research has revolutionized glycomics by enabling comprehensive structural characterization of free glycans and glycoconjugates in a sensitive and high throughput fashion. In the 1980s she was among the first to recognize the potential of combining emerging soft ionization techniques with tandem mass spectrometry for characterization of glycans. Today, her 1988 publication defining the dissociation nomenclature for glycans remains highly cited. Prof. Costello delineated the strategy of producing the greatest degree of structural detail on glycans in a single tandem mass spectrometry step. She recognized that while collisional dissociation provides useful information, its utility is limited by low abundances of key cross-ring cleavage product ions. She developed activated electron dissociation methods for glycans and glycoconjugates that are inherently more effective for producing cross-ring cleavages. This has included studies of dissociation mechanisms and influences of metal cationization. Prof. Costello and her co-workers also pioneered Fourier Transform mass spectrometry of glycans and glycoconjugates with the application of electron based activation/dissociation methods and demonstrated these methods on a time scale compatible with on-line LC-tandem MS. Prof. Costello was the first to demonstrate top-down tandem MS analysis of intact glycoproteins. This is significant because most cell surface and secreted proteins are glycosylated and progress in biomedicine depends on the ability to characterize glycosylated proteoforms.

Prof. Costello's research activities define the present state of the art in glycan and glycoconjugate tandem mass spectrometry. These achievements address the needs in biomedicine for high throughput sequencing of glycans and glycoconjugates and for top-down analysis of intact glycoproteins.

Dr. Catherine E. Costello is a William Fairfield Warren Distinguished Professor, Department of Biochemistry, Cell Biology & Genomics, Department of Physiology & Biophysics, and Department of Chemistry, Boston University, Boston, MA.

RON A. HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, SAGAMORE 5-7, LEVEL 2



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 certificates.

The 2017 Award recognizes Thomas Rizzo, École Polytechnique Fédérale de Lausanne and co-authors for their paper **Infrared Spectroscopy of Mobility-Selected H⁺-Gly-Pro-Gly-Gly (GPGG)**; Antoine Masson¹, Michael Z. Kamrath¹, Marta A. S. Perez¹, Matthew S. Glover², U. Röthlisberger¹, David E. Clemmer², Thomas R. Rizzo¹; ¹École Polytechnique Fédérale de Lausanne, ²Indiana University; JASMS Vol. 26, Sept 2015, pp. 1444-1454



Antoine
Masson



Michael
Kamrath



Marta
Perez



Matthew
Glover



Ursula
Rothlisberger



David
Clemmer



Thomas
Rizzo



BIEMANN MEDAL

2017 RECIPIENT: RYAN JULIAN

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



Dr. Ryan Julian is awarded the 2017 Biemann Medal for contributions related to his work developing and exploiting photo-initiated gas phase radical ion chemistry to probe peptide and protein structure. Several applications that rely on this chemistry have been developed by Ryan's lab including methods for (1) examining 3D protein structure in the gas phase, (2) site specific identification of Ser or Thr phosphorylation, (3) identification of Cys residues and disulfide pairs, (4) identification of peptide epimers, (5) oligosaccharide characterization, and (5) monitoring energy transfer with UV action spectra.

Prof. Julian has developed bond selective chemistry for initiating controllable radical directed dissociation (RDD). This is accomplished by photoexcitation with ultraviolet photons, leading to homolytic dissociation of specific bonds and the generation of a radical species. For example, photodissociation of carbon-iodine bonds with 266 nm photons occurs with high yield due to excitation of a dissociative excited state. If the carbon is covalently attached to a protein, then a radical is generated at that atom, and iodine radical is lost. The Julian lab has demonstrated that this chemistry can be used to create radicals in various types

of biomolecules via dissociation of carbon-iodine, carbon-sulfur, and sulfur-sulfur bonds associated with numerous chromophores. Importantly, any of these bonds can be photodissociated regardless of molecular size, charge state, charge polarity, or sequence. The specificity inherent with this method allows for precise placement of an active radical in a controllable location, which can subsequently initiate fragmentation of the molecule via radical directed dissociation.

Dr. Julian is a professor in the Department of Chemistry at the University of California, Riverside.

2017 RESEARCH AWARDS

AWARD PRESENTATION: 4:45 PM TUESDAY, HALL D, 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

**Peter Nemes***The George Washington University*

Sponsored by

WATERS CORPORATION

**Abraham Badu-Tawiah***The Ohio State University*

AWARDS

2017 POSTDOCTORAL CAREER DEVELOPMENT AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, SAGAMORE 5-7, LEVEL 2

Five 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.



Bushra Amin
*University of
Pittsburgh*



Andrea Carra
*University of
Minnesota*



Romel P. Dator
*University of
Minnesota*



Charles M. Nichols
Vanderbilt University



Wen-Jing Zhang
*Wayne State
University*

2017 STUDENT AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, SAGAMORE 5-7, LEVEL 2

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

Melissa Budelier, Washington University

Bifan Chen, University of Wisconsin-Madison

Bingming Chen, University of Wisconsin-Madison

James Dodds, Vanderbilt University

Paul Hutchins, University of Wisconsin-Madison

Rosemary Onjiko, George Washington University

Elizabeth Peuchen, University of Notre Dame

Lindsay Pino, University of Washington

Matthew Waas, Medical College of Wisconsin

Emily Werth, University of North Carolina

UNDERGRADUATE STUDENT AWARDS

Giovanni Calderisi, University of Innsbruck

Jack Clemmensen, Saint Mary's College of California

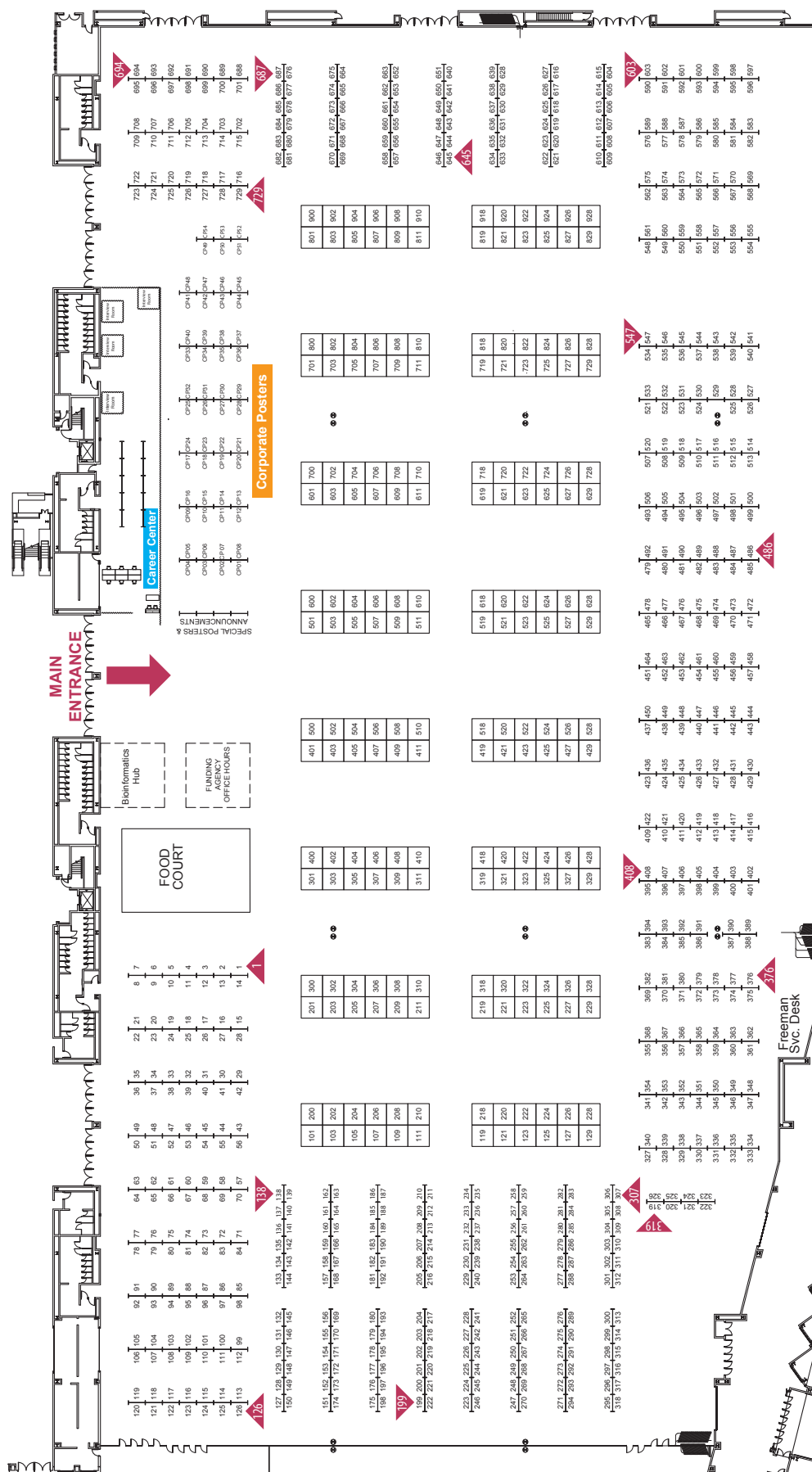
Jason Cochran, University of Florida

Mirna Giron, Kean University

Christopher Gongar, University of Florida

Shilpa Kolachina, University of Illinois at Chicago

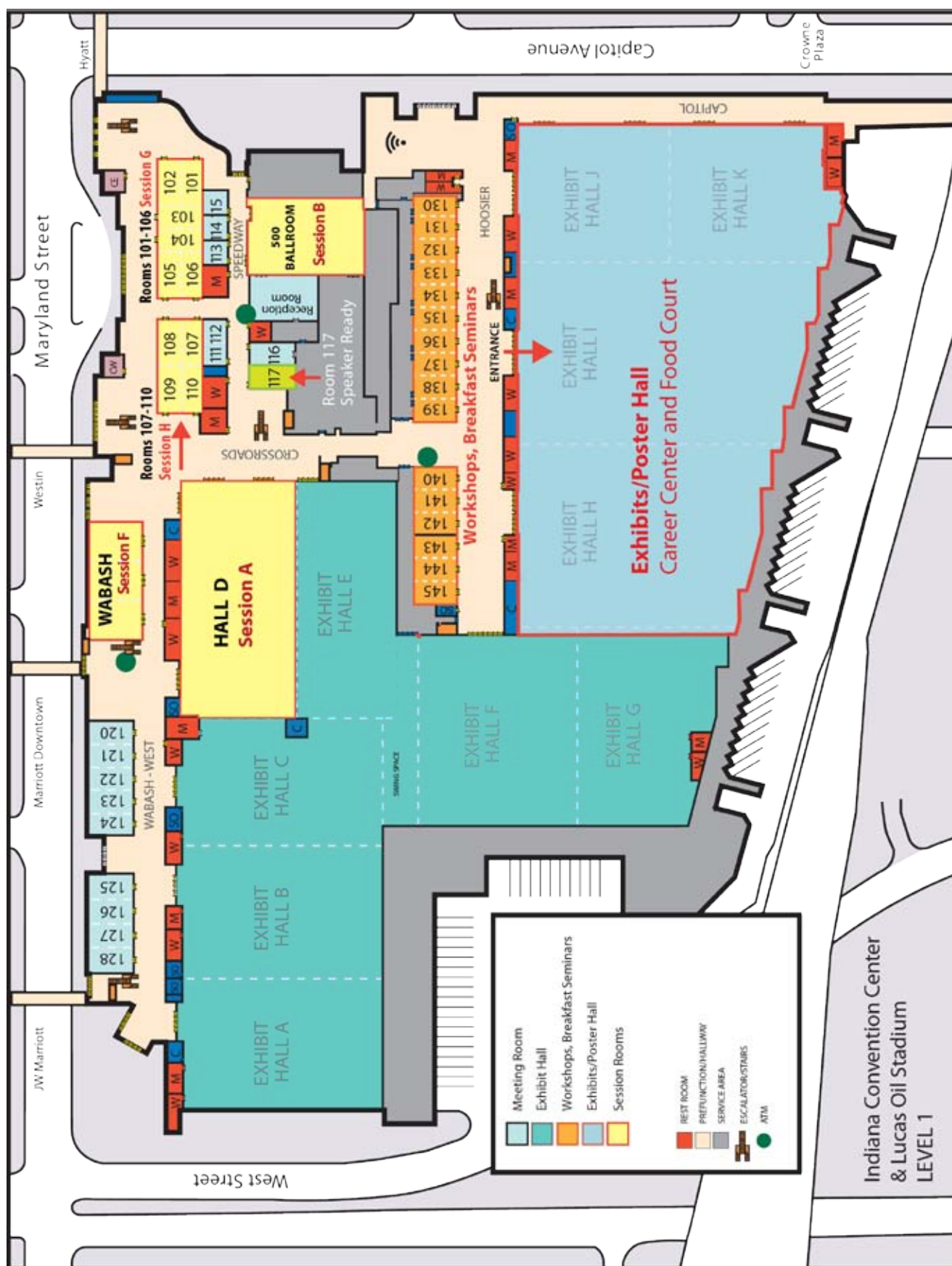
John Lin, University of Texas at Austin





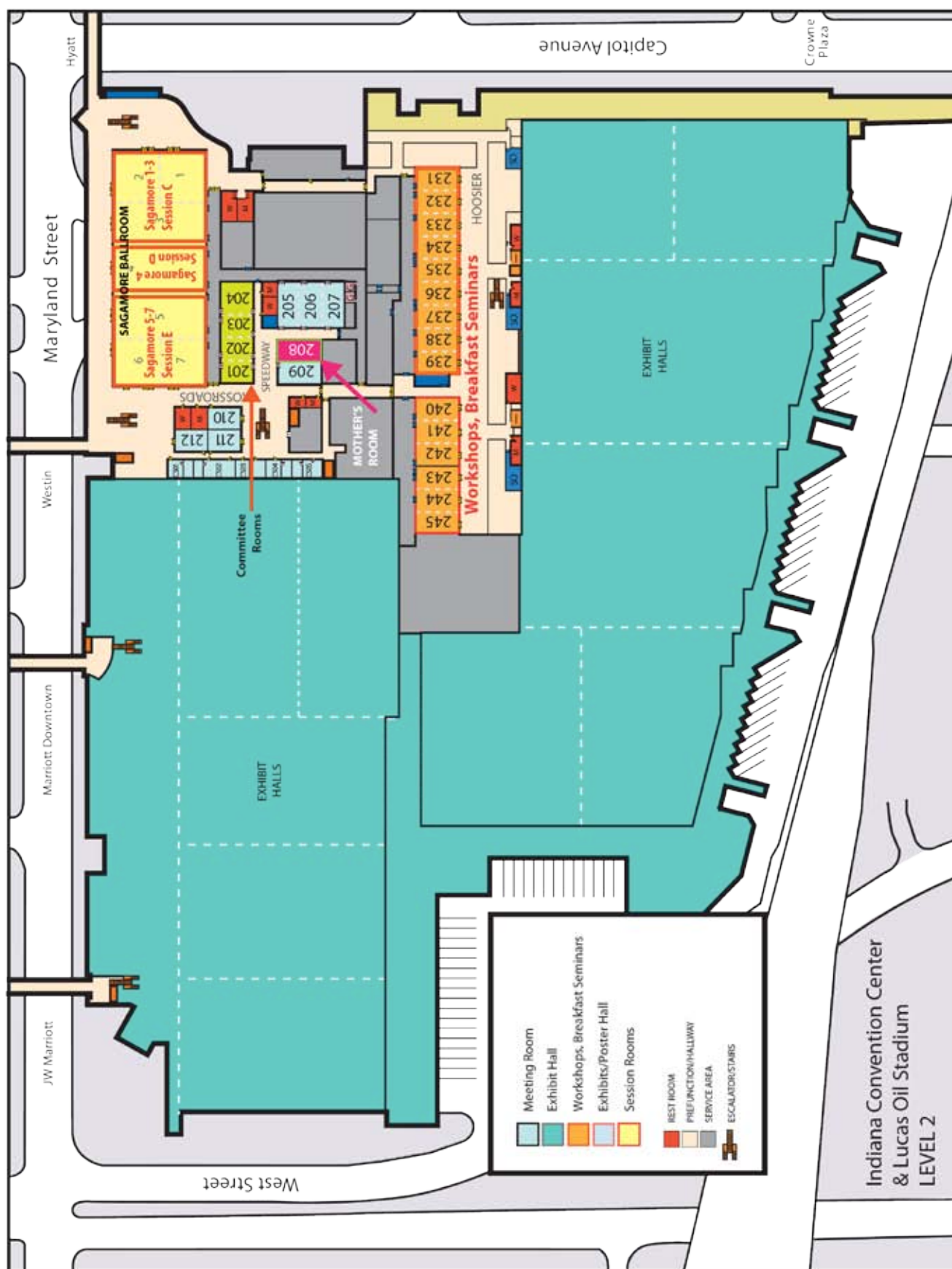
INDIANA CONVENTION CENTER

Level 1






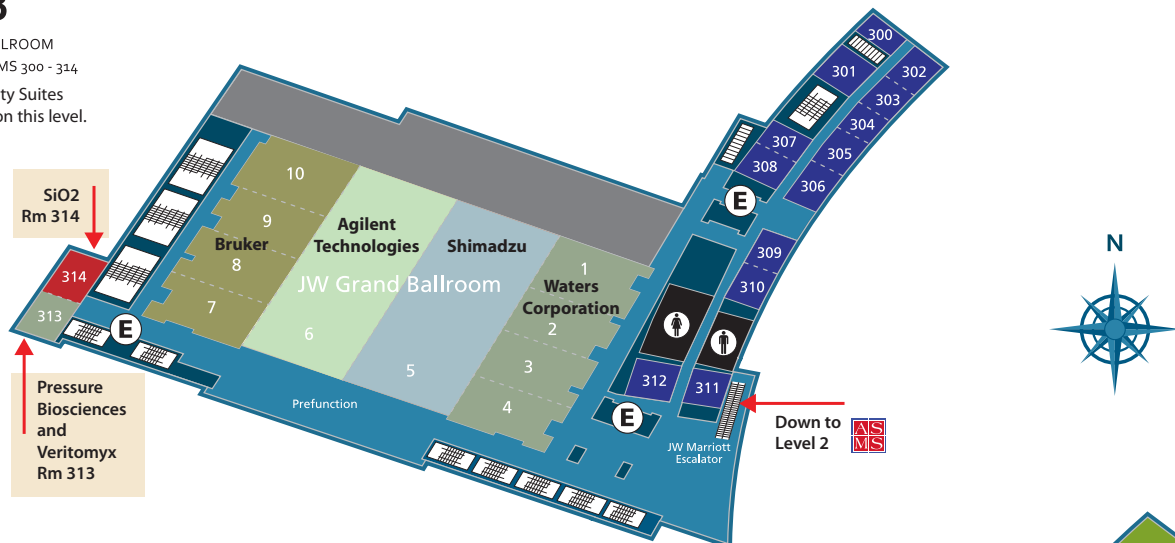
Level 2



LEVEL 3

JW GRAND BALLROOM
MEETING ROOMS 300 - 314


 Hospitality Suites
located on this level.

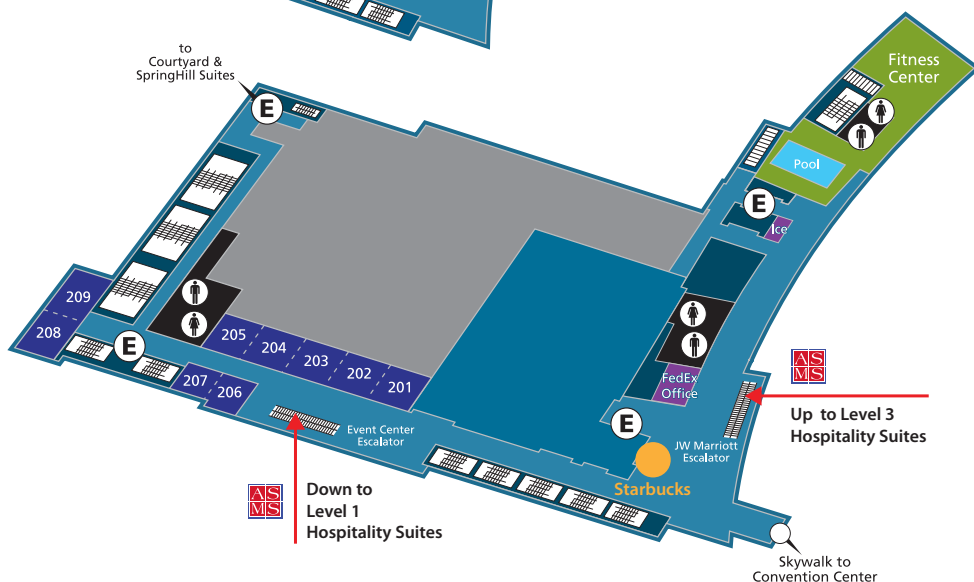


LEVEL 2

ESCALATORS
DOWN TO LEVEL 1
UP TO LEVEL 3

ACCESS to
COURTYARD & SPRINGHILL SUITES
SKYWALK to
CONVENTION CENTER
INDIANAPOLIS MARRIOTT

 Level 2 serves as the access point to Hospitality Suites. From Level 2 guests can take escalators UP to Level 3 suites or down to Level 1 suites.



LEVEL 1


WHITE RIVER BALLROOM
MEETING ROOMS 101 - 109
EVENT CENTER ENTRANCE


 Hospitality Suites
located on this level.

 BALLROOMS / EXHIBIT HALL

 MEETING ROOMS

 FITNESS CENTER / POOL

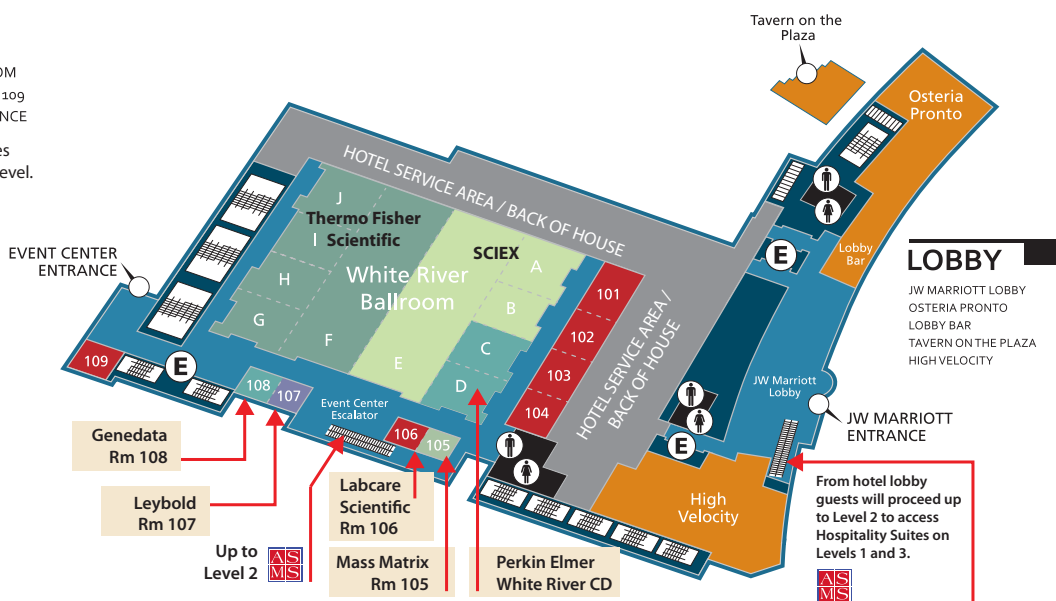
 RESTAURANTS
Osteria Pronto
Lobby Bar
Tavern on the Plaza
High Velocity
T.G.I. FRIDAY'S

 SERVICES
FedEx Office
ICE
Hertz Car Rental - (Level P3 at JW Marriott Garage Elevator)

 ELEVATOR

 RESTROOM - Men

 RESTROOM - Women





HOSPITALITY SUITES 2017 - BACK TO BASICS

ASMS Corporate Member Hospitality Suites return to their roots in Indianapolis. When the hospitality suite concept was first introduced at the conference, the intention was to provide a relaxed atmosphere where attendees could interact with industry. To provide a setting for meaningful conversations regarding the latest technology in products and services, and attendees could network and enjoy refreshments.

In Indianapolis, hospitality suites will embrace the back to basics atmosphere which will allow attendees to learn more about Corporate Member products and services while enjoying fun, food, drink – and *conversation*.

Conference name badges are required for access to all conference activities including hospitality suites.

MEDIA EVENTS (PRESS CONFERENCES)

The following media events are scheduled **Monday, June 5** in the JW Marriott Hotel. All press are invited to attend these events.

8:00 - 9:00 am	Shimadzu Scientific Instruments	Grand Ballroom 5
9:30 - 10:30 am	Bruker Daltonics	Grand Ballroom 7-9
11:00 am - 12:00 pm	SCIEX	White River EAB
1:30 - 2:30 pm	Agilent Technologies	Grand Ballroom 6
3:00 - 4:00 pm	Thermo Fisher Scientific	White River F-J
4:30 - 5:30 pm	Waters Corporation	Grand Ballroom 1-4

BREAKFAST SEMINARS

Breakfast seminars are hosted by corporate members at either the Convention Center or the JW Marriott Hotel (inside hospitality suites). Pre-registration is recommended because room set-up and catering are arranged in advance. Please look for Breakfast Seminars page on www.asms.org and in the mobile app to find online registration links.

MONDAY BREAKFASTS	CONVENTION CENTER <i>Start times vary, see below.</i>	
	Advanced Chemistry Development	Room 140, 6:45 am
	LECO Corporation	Room 139, 6:45 am
	Matrix Science	Room 137-138, 7:00 am
	Perkin Elmer	Room 130, 7:00 am
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	Waters Corporation	Room 133-134, 7:00 am
	JW MARRIOTT HOTEL <i>Start times vary, see below.</i>	
	Agilent Technologies	Grand Ballroom 6, 7:00 am
	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific (2)	White River F and GH, 7:00 am
TUESDAY BREAKFASTS	Waters Corporation	Grand Ballroom 1-4, 7:00 am
	CONVENTION CENTER <i>Start times vary, see below.</i>	
	Biognosys	Room 130, 7:00 am
	LECO Corporation	Room 139, 6:45 am
	Matrix Science	Room 137-138, 7:00 am
	New Objective	Room 239, 6:45 am
	NIST Mass Spectrometry Data Center John Wiley and Sons Publishers	Room 141-142, 7:00 am
	Prosolia	Room 240, 7:00 am
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	SYFT	Room 245, 7:00 am
	Waters Corporation	Room 133-134, 7:00 am
	JW MARRIOTT HOTEL <i>Start times vary, see below.</i>	
	Agilent Technologies	Grand Ballroom 6, 7:00 am
	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific (2)	White River F and GH, 7:00 am
	Waters Corporation	Grand Ballroom 1-4, 7:00 am

WEDNESDAY BREAKFASTS	CONVENTION CENTER <i>Start times vary, see below.</i>	
	LECO Corporation	Room 139, 6:45 am
	New Objective	Room 130, 6:45 am
	SCIEX (3)	Rms 140, 143-144, and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	JW MARRIOTT HOTEL <i>Start times vary, see below.</i>	
	Agilent Technologies	Grand Ballroom 6, 7:00 am
THURSDAY BREAKFASTS	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific	White River F and GH, 7:00 am
	Waters Corporation	Grand Ballroom 1-4, 7:00 am
	CONVENTION CENTER <i>Start times vary, see below.</i>	
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	Thermo Fisher Scientific	Room 141-142, 7:00 am





CORPORATE MEMBERS

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
908 Devices	200			
AcroMass Technologies	729	Corporate Poster		
Advanced Chemistry Development (ACD/Labs)	711	Corporate Poster		Conv Ctr Rm 140: Mon 6/5
Advanced Chromatography Technologies, Ltd	101			
Advanced Energy	400	Corporate Poster		
Advion Inc.	506			
Agilent Technologies	600	Corporate Poster	Grand Ballroom 6	JW Marriott Grand 6: Mon-Wed (6/5-6/7)
American Chromatography Supplies	405			
Analytical Sales and Services, Inc.	605	Corporate Poster		
Anest Iwata	708			
Antec	519	Corporate Poster		
Apricot Designs, Inc.	303			
Ardara Technologies LP	324			
ASTA	421	Corporate Poster		
Avanti Polar Lipids, Inc.	928			
Baran Bioscience, LLC		Corporate Poster		
BioChromato, Inc.	821			
BIOCRATES Life Sciences AG	904			
Biognosys	507			Conv Ctr Rm 130: Tue 6/6
Bioinformatics Solutions Inc.	508	Corporate Poster		
Biopeptek, Inc	622			
Biotage	528			
Bonna-Agela Technologies, Inc.	227			
Bruker Daltonics	518		Grand Ballroom 7-10	JW Marriott Grand 10: Mon-Wed (6/5-6/7)
C&EN		Publisher Tabletop		
Cambridge Isotope Labs	618			
Cayman Chemical Company	803			
CDS Analytical	722			
CEM Corporation	619			
Cerno Bioscience	628			
Chemyx, Inc.	806			
CMP Scientific, Inc.	828			
Compare Networks		Publisher Tabletop		
CovalX	626			
CSS Analytical Co. Inc.	420			
CTC Analytics AG	607			
Detector Technology, Inc.	219			
Digital Proteomics	704			
Dikma Technologies, Inc	228			
Drummond Scientific	720			

CORPORATE MEMBERS



	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
EBARA Technologies	702			
Edwards Vacuum	707			
El-Mul Technologies	721			
e-MSion, Inc.	723			
Entech Instruments	918	Corporate Poster		
ESI Source Solutions	429			
ETP Electron Multipliers/Ion Detect	424	Corporate Poster		
Excellims Corporation	404			
Extrel	719			
Fasmatech	726			
FLIR Systems, Inc.	709			
Genedata	510	Corporate Poster	Room 108	
Genetic Engineering & Biotechnology News		Publisher Tabletop		
Genovis	706			
GenTech Scientific, Inc.	428			
GERSTEL, Inc.	524	Corporate Poster		
GL Sciences Inc.	401			
Grenova	724			
Hamamatsu Corporation	725			
Hamilton Company	810	Corporate Poster		
Harris Corp	418			
HILICON		Corporate Poster		
Horizon Technology, Inc.	727			
HTX Technologies, LLC	426			
IDEX Health & Science	411	Corporate Poster		
IMCS	201	Corporate Poster		
Imtakt USA	610			
InstruTech	224			
INTAVIS Bioanalytical Instruments AG	308			
Integrated Proteomics Applications	226			
International Ceramic Engineering	323			
International Equipment Trading Ltd.	504			
International Labmate		Publisher Tabletop		
Intertek Pharmaceutical Services	629			
ionBench	419			
Ionoptika Ltd	322			
IonSense, Inc.	718	Corporate Poster		
ION-TOF GmbH	425			
IsoSciences	203			
JASMS	111			
Jaytee Biosciences Ltd	302			
JEOL USA, Inc.	801			
Jordi Labs	423	Corporate Poster		
Kashiyama USA	804			



CORPORATE MEMBERS

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Knauer Wissenschaftliche Geräte GmbH	620			
Labcare Scientific International	205		Room 106	
Labcyte		Corporate Poster		
LECO Corporation	603	Corporate Poster		Conv Ctr Rm 139: Mon-Wed 6/5-6/7
Leybold USA Inc	525		Room 107	
Linden CMS GmbH	407			
MasCom Technologies	326			
MassMatrix		Corporate Poster	Room 105	
MassTech Inc.	327			
Matrix Science	328			Conv Ctr Rm 137-138: Mon 6/5, Tue 6/6
McKinley Scientific	606			
MeCour Temperature Control	229			
Mestrelab Research, S.L.	505			
MilliporeSigma	805			
Moeller Medical GmbH	521			
MPF Products Inc	210			
MRM Proteomics Inc	827			
MS Ekspert	320			
MS Noise	529			
MS Vision (Spectrometry Vision B.V.)	406			
mSPEC group	223			
MStm	705			
Nacalai USA, Inc.	829	Corporate Poster		
nanoLiter, LLC	209	Corporate Poster		
Navac LLC	808			
Nest Group, The		Corporate Poster		
New England Biolabs	908			
New England Peptide, Inc.	422			
New Objective, Inc.	604	Corporate Poster		Conv Ctr Rm 239: Tue 6/6, Conv Ctr Rm 130: Wed 6/7
NewOmics, Inc	809			
NIST	700			Conv Ctr Rm 141-142: Tue 6/6
Novilytic	609			
Omicron Biochemicals	509	Corporate Poster		
Omics, LLC	306	Corporate Poster		
Omni International	811			
Optimize Technologies, Inc.	403	Corporate Poster		
Owlstone Medical Ltd.	325			
Pace Analytical	119			
Parker Balston/Hannifin	409			
PEAK Scientific	701	Corporate Poster		

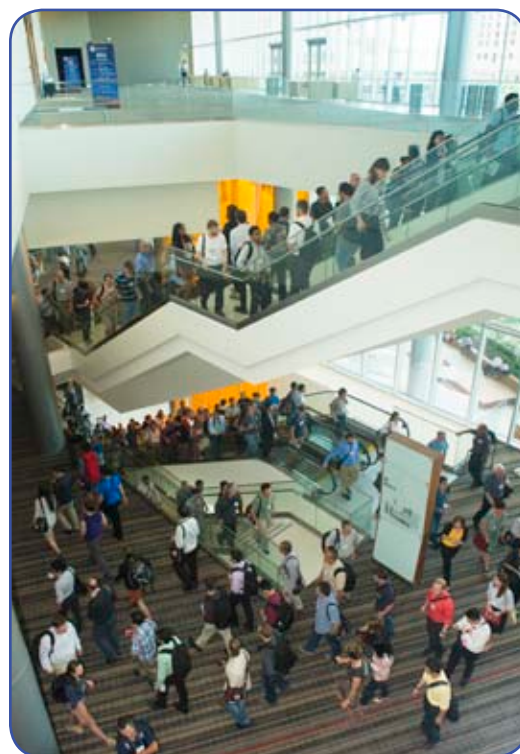
CORPORATE MEMBERS



	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Perfinity Biosciences	523			
PerkinElmer	319		White River CD	Conv Ctr Rm 130: Mon 6/5
Pfeiffer Vacuum	301	Corporate Poster		
PharmaFluidics	225	Corporate Poster		
Phenomenex	627			
Phoenix S&T, Inc.	520			
PHOTONIS	300	Corporate Poster		
Physical Electronics	910	Corporate Poster		
Phytronix Technologies, Inc.	211			
Polymer Factory Sweden AB	310	Corporate Poster		
Postnova	608	Corporate Poster		
Presco Incorporated	202			
Pressure BioSciences, Inc.	329	Corporate Poster	Room 313	
Prolab Instruments GmbH	825			
Promega Corporation	800			
Prosolia, Inc.	611	Corporate Poster		Conv Ctr Rm 240: Tue 6/6
Protea Biosciences, Inc.	305			
Protein Metrics Inc.	410			
Proteome Software Inc.	218			
ProteoWorker	307	Corporate Poster		
Proton Onsite	621			
Prozyme, Inc.	427			
PURSPEC Technologies, Inc.	623			
Resolution Labs LLC	526			
Restek Corporation	900			
ReSyn Biosciences	408	Corporate Poster		
Samin Science Co., Ltd	129			
Science/AAAS		Publisher Tabletop		
Scientific Instrument Services	503	Corporate Poster		
Scientific Systems, Inc.	204			
SCIEX	500		White River EAB	Conv Ctr Rm 140: Wed 6/7 Conv Ctr Rm 143-144: Mon-Thur 6/5-6/8 Conv Ctr Rm 145: Mon-Thur 6/5-6/8
SepSolve Analytical	220			
Shimadzu Scientific Instruments, Inc.	511	Corporate Poster	Grand Ballroom 5	Conv Ctr Rm 135-136: Mon-Thur 6/5-6/8
Sierra Analytics	802	Corporate Poster		
Silantes GmbH	304			
SiO2 Medical Products	321		Room 314	
Sound Analytics	625			
Spark Holland	820			
SpectralWorks Limited	522	Corporate Poster		
Spectroscopy	822			
Spectroswiss	710			

CORPORATE MEMBERS

Company	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Spellman High Voltage	818			
SPEX SamplePrep	207			
SunChrom GmbH	819			
Superior Technical Ceramics	221			
SYFT Technologies	402	Corporate Poster		Conv Ctr Rm 245: Tue, 6/6
The Analytical Scientist		Publisher Tabletop		
Thermo Fisher Scientific	601		White River F-J	Conv Ctr Rm 141-142: Thu 6/8 JW Marriott White River F & GH: Mon-Wed 6/5-6/7
Tofwerk AG	624			
Tosoh Bioscience	728			
Trajan Scientific and Medical	703	Corporate Poster		
Veritomyx	318	Corporate Poster	Room 313	
VICI Valco Instruments	824			
VRS	602			
VUV Analytics	311			
Waters Corporation	501	Corporate Poster	Grand Ballroom 1-4	Conv Ctr Rm 133-134: Mon-Tues 6/5-6/6 JW Marriott Grand 1-4: Mon-Wed 6/5-6/7
Wiley		Publisher Tabletop		Conv Ctr Rm 141-142: Tue 6/6
XPC Corporation	502			
Zef Scientific Inc.	309			
Zhejiang Haochuang Biotech Co., Ltd	826			



PROGRAM ACKNOWLEDGEMENTS

VICE PRESIDENT FOR PROGRAMS



Richard A. Yost
University of Florida
Vice President for Programs

STUDENT ASSISTANTS

Graduate students and postdoctoral fellows 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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	Cheng Lin	Salvatore Sechi	



PROGRAM OVERVIEW

SATURDAY

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

SUNDAY

9:00 AM - 4:30 PM	SHORT COURSES
10:00 AM - 8:00 PM	REGISTRATION
4:00 - 4:45 PM	ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS, Room 107-110 level 1
5:00 - 6:30 PM	<p>TUTORIAL LECTURES, Hall D level 1</p> <div> <div> <p>5:00 - 5:45 pm MALDI: Past and Future Kermit K. Murray, <i>Louisiana State University</i></p>  </div> <div> <p>5:45 - 6:30 pm Cancer Immunotherapy and Mass Spectrometry Donald F. Hunt, <i>University of Virginia</i></p>  </div> </div> <div> <div> <p>TUTORIAL SESSION II, Wabash level 1 5:00 - 5:45 pm Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life Erin S. Baker, <i>Pacific Northwest National Lab</i></p>  </div> <div> <p>5:45 - 6:30 pm CE/MS -Ready for Prime Time? Norman J. Dovichi, <i>University of Notre Dame</i></p>  </div> </div>
6:45 - 7:45 PM	<p>CONFERENCE OPENING, Hall D level 1 Richard A. Yost, <i>University of Florida</i> <i>ASMS Vice President for Programs</i></p> <div>  <div> <p>7:00 - 7:45 pm Towards a Good Start in Life: Neonatal Screening and Beyond David S. Millington <i>Duke University Medical Center</i></p> </div> </div>
7:45 - 9:00 PM	WELCOME RECEPTION IN THE POSTER/EXHIBIT HALL Undergraduate Student Poster Competition

PROGRAM OVERVIEW



MONDAY

FROM 6:45 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS MOA am: Celebration of Klaus Biemann's Science, <i>Hall D level 1</i> MOB am: Applications of Stable Isotope Labeling in MS, <i>500 Ballroom level 1</i> MOC am: Metabolomics: New Technologies and Applications, <i>Sagamore 1-3 level 2</i> MOD am: Innovations and Applications in Forensics, <i>Sagamore 4 level 2</i> MOE am: Plant "omics", <i>Sagamore 5-7 level 2</i> MOF am: Ion Mobility: New Developments and Applications, <i>Wabash level 1</i> MOG am: Instrumentation: New Developments in Ion Detection, <i>Room 101-106 level 1</i> MOH am: Synthetic Polymers, <i>Room 107-110 level 1</i>
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Monday Posters, Poster/Exhibit 11:30 am - 1:00 pm: Undergraduate students – look for reserved tables and free lunch vouchers to Meet the Experts
2:30 - 4:30 PM	ORAL SESSIONS MOA pm: MS in Clinical Analysis, <i>Hall D level 1</i> MOB pm: Analytical Challenges of Microdosing and Microsampling Studies, <i>500 Ballroom level 1</i> MOC pm: Metabolomics: Untargeted Profiling, <i>Sagamore 1-3 level 2</i> MOD pm: Environmental: Emerging Contaminants, <i>Sagamore 4 level 2</i> MOE pm: Hydrogen-Deuterium Exchange MS, <i>Sagamore 5-7 level 2</i> MOF pm: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, <i>Wabash level 1</i> MOG pm: Instrumentation: Ambient Ionization: Instrumentation & Applications, <i>Rm 101-106 level 1</i> MOH pm: Fundamentals: Ion-Ion and Ion-Neutral Interactions, <i>Room 107-110 level 1</i>
4:45 - 5:30 PM	AWARD LECTURE , Hall D level 1 Award for a Distinguished Contribution in Mass Spectrometry  Catherine E. Costello <i>Boston University</i>
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas. 01. Improving Scientific Writing Skills, <i>Room 130 level 1</i> 02. Metal Ion Coordination in Gas-Phase Bioanalysis: Reaping Practical Benefits (Metal Ion Coordination Chemistry Interest Group), <i>Room 131-132 level 1</i> 03. Open Source Software Packages: Using and Making your Contributions (Bioinformatics MS Interest Group), <i>Room 133-134 level 1</i> 04. Clinical Diagnostics: Translating New Mass 8. Spectrometry Approaches (Clinical Chemistry Interest Group), <i>Room 135-136 level 1</i> 05. FTMS: Successes and Challenges of Achieving Routinely High Mass Accuracy (FTMS Interest Group), <i>Room 137-138 level 1</i> 06. Exposomics Update: Success, Lessons and Future Goals (Exposomics Interest Group), <i>Room 139 level 1</i> 08. Antibody-Drug Conjugate Research and Development: The Role of Multifaceted Mass Spectrometry (Pharmaceuticals Interest Group), <i>Room 141-142 level 1</i> 09. Forensics and Homeland Security Mass Spectrometry Research: A Critical Discussion between Academicians and Forensic Science Practitioners (Forensics & Homeland Security Interest Group), <i>Room 143-144 level 1</i> 10. Art and Cultural Heritage: Mass Spec Applications, <i>Room 145 level 1</i> 11. Mass Spectrometry Interactive Virtual Environment (MassIVE): Management of Big Data, <i>Room 231-234 level 2</i> 12. Ion Trap Instrumentation for Harsh Environment and Point-of-Care Applications (Ion Trap MS Interest Group), <i>Room 235-238 level 2</i> 13. Photoionization: Applications, Developments, and Discussions (Photoionization MS Interest Group), <i>Room 239 level 2</i> 14. A Career in Mass Spec: Options and Where to start? (Young Mass Spectrometrists Interest Group), <i>Room 240-242 level 2</i> 15. Top-Down Proteomics, <i>Room 243-245 level 2</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , JW Marriott Hotel

PROGRAM OVERVIEW

TUESDAY

FROM 6:45 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS TOA am: Informatics: Peptide and Protein Identification, <i>Hall D level 1</i> TOB am: Quantitative Analysis in Drug Discovery and Development, <i>500 Ballroom level 1</i> TOC am: Qualitative and Quantitative Analysis of PTMs, <i>Sagamore 1-3 level 2</i> TOD am: Exposomics: Targeted, Untargeted and Bioinformatics Methodologies, <i>Sagamore 4 level 2</i> TOE am: Macromolecular Complexes, <i>Sagamore 5-7 level 2</i> TOF am: Ion Mobility: Structure, <i>Wabash level 1</i> TOG am: Instrumentation: Mass Analyzer Innovations, <i>Room 101-106 level 1</i> TOH am: Fundamentals: Ion Spectroscopy, <i>Room 107-110 level 1</i>
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Tuesday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	ORAL SESSIONS TOA pm: Informatics: Metabolomics, <i>Hall D level 1</i> TOB pm: MS in the Regulatory Environment, <i>500 Ballroom level 1</i> TOC pm: Quantitative Proteomics in Systems Biology, <i>Sagamore 1-3 level 2</i> TOD pm: Environmental: New Instrumentation and Approaches, <i>Sagamore 4 level 2</i> TOE pm: Covalent Labeling and Chemical Crosslinking, <i>Sagamore 5-7 level 2</i> TOF pm: Microorganisms: Identification and Characterization, <i>Wabash level 1</i> TOG pm: Instrumentation: Innovations in FT-based Mass Analyzers, <i>Room 101-106 level 1</i> TOH pm: Fundamentals: Ion Activation and Dissociation, <i>Room 107-110 level 1</i>
4:45 - 5:30 PM	AWARD LECTURE , Hall D level 1 Biemann Medal  Ryan Julian <i>University of California, Riverside</i>
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas. 01. Trans-Proteomic Pipeline: New Advances and Future Developments, <i>Room 130 level 1</i> 02. Bioinformatic Approaches for Glycomics/ Glycoproteomics, <i>Room 131-132 level 1</i> 03. Statistics and Bioinformatics using R, <i>Room 133-134 level 1</i> 04. Environmental Analysis: Modern Sampling Techniques and Data Analysis (Environmental Applications Interest Group), <i>Room 135-136 level 1</i> 05. Hepatocytes: Current and Future Use in DMPK (DMPK Interest Group), <i>Room 137-138 level 1</i> 06. The NIH and NSF Review and Funding Process, <i>Room 139 level 1</i> 07. Proteomic Workflow: Unpublished Collective Practical Knowledge from Insiders (Analytical Lab Managers Interest Group), <i>Room 140 level 1</i> 08. The Need for Speed: Is your LC or Mass Spectrometer the Top Gun for Improving Throughput? (LCMS & Related Topics Interest Group), <i>Room 141-142 level 1</i> 09. Tracing Uncertainty in Imaging MS: Benchmarking Reproducibility, Variability, and Performance across Experiments (Imaging MS Interest Group), <i>Room 143-144 level 1</i> 10. JASMS - Present Status and Future, <i>Room 145 level 1</i> 11. Biotherapeutics: Hot Topics (Biotherapeutics Interest Group), <i>Room 231-234 level 2</i> 12. HDX, Covalent Labeling & Cross Linking: State-of-the-Art and Future Directions (HDX Covalent Labeling & Cross Linking Interest Group), <i>Room 235-238 level 2</i> 13. Polymer Mass Spectrometry: Advances (Polymeric Materials Interest Group), <i>Room 239 level 2</i> 14. Metabolomics: Integration into the Emerging Arena of Multi-omic Approaches (Metabolomics Interest Group), <i>Room 240-242 level 2</i> 15. Mass Spectrometry and Ion Mobility: The Role of Temperature (Fundamentals Interest Group), <i>Room 243-245 level 2</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , JW Marriott Hotel

PROGRAM OVERVIEW



WEDNESDAY

FROM 6:45 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS WOA am: Informatics: DIA: Innovative Methods and Applications, <i>Hall D level 1</i> WOB am: Food Safety & Chemistry: Non-targeted Screening, <i>500 Ballroom level 1</i> WOC am: Biomarkers: Qualitative Analysis, <i>Sagamore 1-3 level 2</i> WOD am: Lipidomics: Lipids and Profiling, <i>Sagamore 4 level 2</i> WOE am: Glycopeptides and Glycoproteins, <i>Sagamore 5-7 level 2</i> WOF am: Imaging: Instrumentation & Method Development, <i>Wabash level 1</i> WOG am: Instrumentation: MS in Extreme Environments, <i>Room 101-106 level 1</i> WOH am: Fundamentals: Photoionization and Photodissociation, <i>Room 107-110 level 1</i>
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Wednesday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	ORAL SESSIONS WOA pm: Informatics: Multiomics Integration and Applications, <i>Hall D level 1</i> WOB pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, <i>500 Ballroom level 1</i> WOC pm: Antibodies and Antibody Drug Conjugates, <i>Sagamore 1-3 level 2</i> WOD pm: Lipidomics: New MS Technologies and Applications, <i>Sagamore 4 level 2</i> WOE pm: Biomarkers: Quantitative Analysis, <i>Sagamore 5-7 level 2</i> WOF pm: Imaging: Computational Methods and Analysis, <i>Wabash level 1</i> WOG pm: Instrumentation: New Developments in Ionization and Sampling, <i>Room 101-106 level 1</i> WOH pm: Fundamentals: Molecular Modeling and Quantum Mechanical Calculations in Ion Mobility and MS, <i>Room 107-110 level 1</i>
4:45 - 5:30 PM	ASMS MEETING , Sagamore 5-7 level 2: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	WORKSHOPS There are light refreshments in the common areas. 01. Career and Collaboration Opportunities in China, <i>Room 130 level 1</i> 02. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: New Trends, <i>Room 131-132 level 1</i> 03. Diversity and Outreach, <i>Room 133-134 level 1</i> 04. Galaxy-P in the Cloud: Proteomic Informatics on JetStream, <i>Room 135-136 level 1</i> 05. Food Safety & Authenticity: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group), <i>Room 137-138 level 1</i> 06. Energy, Petroleum, and Biofuels: Experimental Challenges (Energy Petroleum & Biofuels Interest Group), <i>Room 139 level 1</i> 07. Undergraduate Research in Mass Spectrometry: Making the Most of It (Undergraduate Research in MS Interest Group), <i>Room 140 level 1</i> 08. Quantitative Glycomics and Glycoproteomics, <i>Room 141-142 level 1</i> 09. Mass Spectrometry in GMP Environment: Aspects of System Qualification and Method Validation, <i>Room 143-144 level 1</i> 10. Mass Spectrometry in the Developing World: Supporting Education and Research, <i>Room 145 level 1</i> 11. Lipidomics Data Processing and Analyses: Software Tools (Lipids & Lipodomics Interest Group), <i>Room 231-234 level 2</i> 12. Data Independent Acquisition Strategies for Quantitative Proteomics: The Challenges of Scaling Up to Meet Demand (Data Independent Acquisition Interest Group), <i>Room 235-238 level 2</i> 13. Nucleic Acid-based Therapeutics: Structure Identification and Bioanalysis (Oligonucleotides and Nucleic Acids Interest Group), <i>Room 239 level 2</i> 14. Ion Mobility Spectrometry: Towards Standard Operating Procedures (Ion Mobility MS Interest Group), <i>Room 240-242 level 2</i> 15. Bioanalysis of Biosimilars (Regulated Bioanalysis Interest Group), <i>Room 243-245 level 2</i>
7:00 - 8:00 PM	DINNER BREAK
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES , JW Marriott Hotel



PROGRAM OVERVIEW

THURSDAY

FROM 6:45 AM	CORPORATE BREAKFAST SEMINARS , Convention Center (schedule on page 15)
7:30 AM - 5:00 PM	REGISTRATION
8:30 - 10:30 AM	ORAL SESSIONS ThOA am: Informatics: Innovations, <i>Hall D level 1</i> ThOB am: MS in the QC Lab, <i>500 Ballroom level 1</i> ThOC am: Membrane Protein MS, <i>Sagamore 1-3 level 2</i> ThOD am: Nucleic Acids and Oligonucleotides, <i>Sagamore 4 level 2</i> ThOE am: Native MS in Structural Biology, <i>Sagamore 5-7 level 2</i> ThOF am: Imaging: Pharmaceuticals, Metabolites, and Lipids, <i>Wabash level 1</i> ThOG am: GC/MS, GC/GC/MS, GC/MS/MS, and GC/HRMS, <i>Room 101-106 level 1</i> ThOH am: Fundamentals for Everyone, <i>Room 107-110 level 1</i>
10:30 AM - 2:30 PM	POSTER SESSION AND EXHIBITS , Thursday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	ORAL SESSIONS ThOA pm: Informatics: Discovery Proteomics, <i>Hall D level 1</i> ThOB pm: HRMS for Quantitation in Drug Discovery, Development & Beyond, <i>500 Ballroom level 1</i> ThOC pm: Top Down Protein Analysis, <i>Sagamore 1-3 level 2</i> ThOD pm: Carbohydrates, <i>Sagamore 4 level 2</i> ThOE pm: Protein-Ligand Interactions, <i>Sagamore 5-7 level 2</i> ThOF pm: Imaging: Biomedical Applications, <i>Wabash level 1</i> ThOG pm: Instrumentation: Separations Approaches Coupled to MS, <i>Room 101-106 level 1</i> ThOH pm: Energy, Petroleum, and Biofuels: Instrumentation & Applications, <i>Room 107-110 level 1</i>
4:45 - 5:30 PM	PLENARY LECTURE , Hall D level 1 <div data-bbox="376 959 553 1180" data-label="Image"> </div> <div data-bbox="587 1001 930 1033" data-label="Section-Header"> <h4>Saving the Great Coral Reefs</h4> </div> <div data-bbox="587 1058 882 1115" data-label="Text"> <p>Kristen Marhaver <i>Research Station Carmabi</i></p> </div>
6:30 - 9:00 PM	CLOSING EVENT AT THE INDIANA STATE MUSEUM Advance purchase ticket required. The museum is located in the park-like area behind the JW Marriott Hotel complex, an easy walk from convention center and downtown hotels.



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 Marzluff (Grinnell College) and
 JC Poutsma (College of William & Mary)
 Room 107-110 level 1

5:00-6:30 pm Sunday
TUTORIAL SESSION I
 Richard A. Yost (University of Florida)
 Hall D level 1



5:00-5:45 pm
MALDI: Past and Future
Kermit K. Murray
 Louisiana State University



5:45-6:30 pm
Cancer Immunotherapy and Mass Spectrometry
Donald F. Hunt
 University of Virginia

5:00-6:30 pm Sunday
TUTORIAL SESSION II
 John A. McLean (Vanderbilt University)
 Wabash level 1



5:00-5:45 pm
Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life
Erin S. Baker
 Pacific Northwest National Laboratory



5:45- 6:30 pm
CE/MS - Ready for Prime Time?
Norman J. Dovichi
 University of Notre Dame

6:45-7:45 pm Sunday
Conference Opening
 Richard A. Yost (University of Florida)
 Hall D level 1

Welcome, Richard A. Yost, University of Florida
 ASMS Vice President for Programs



7:00-7:45 pm
Towards a Good Start in Life: Neonatal Screening and Beyond
David S. Millington
 Duke University Medical Center

7:45-9:00 pm Sunday
WELCOME RECEPTION
Poster/Exhibit Hall
 Conference name badge is required.



MONDAY MORNING ORAL SESSIONS

From 6:45 am Monday
CORPORATE BREAKFAST SEMINARS
 Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Monday
CELEBRATION OF KLAUS BIEMANN'S SCIENCE
 Dominic Desiderio (Univ. of Tennessee Health Science)
 Hall D level 1

- MOA am 08:30 **A Son's Perspectives on Klaus Biemann's Life;** Hans-Peter Biemann; Sanofi Genzyme, Cambridge, MA
- MOA am 08:50 **Who Invented GC/MS?** Ronald A. Hites; Indiana University, Bloomington, IN

- MOA am 09:10 **Identification of Tumor Specific, Class I MHC Peptides for Immunotherapy of Cancer: Instrumentation and Methods for Characterization of Intact Proteins;** Donald F. Hunt; University of Virginia, Charlottesville, VA
- MOA am 09:30 **A Career of Lipid Biochemistry and Mass Spectrometry: From Fatty Acids to Lipidomics;** Robert C. Murphy; Univ of Colorado Denver, Aurora, CO
- MOA am 09:50 **New Approaches for Localization of Proteins and Interaction Partners in Cells with High Spatial Resolution;** Steven A. Carr; Broad Institute, Cambridge, MA
- MOA am 10:10 **CSI@MIT: Adventures in the Biemann Laboratory;** Catherine E. Costello; Boston University School of Medicine, Boston, MA



MONDAY MORNING ORAL SESSIONS

8:30-10:30 am Monday

APPLICATIONS OF STABLE ISOTOPE LABELING IN MS

Teresa Fan (University of Kentucky)

500 Ballroom level 1

- MOB am 08:30 **Unveiling Metabolic Origins of Cell Surface Glycosylation and Turnover Kinetics of Glycoproteins Using ^{13}C -labeled Saccharides and LC-MS/MS Analysis;** Gege Xu¹; Maurice Wong¹; Qiongyu Li¹; Mariana Barboza¹; Dayoung Park¹; Zhi Cheng¹; Carlito B. Lebrilla¹; ¹University of California, Davis, Davis, California
- MOB am 08:50 **Turnover Measurements of Low Abundance Proteins in Human Plasma and PBMCs by Serial Immunoaffinity and Mass Spectrometry;** Vahid Farrokhi¹; Teresa Caiazzo¹; Katherine Wright¹; Dnise O'Hara¹; Hendrik Neubert¹; ¹Pfizer, Inc., Andover, MA
- MOB am 09:10 **Influence of the Gut Microbiota on Histone Modifications in Intestinal Epithelial Cells;** Peder J. Lund¹; Sarah A. Smith²; Johayra Simithy¹; Zuo-Fei Yuan¹; Kevin A. Janssen¹; Gary D. Wu²; Benjamin A. Garcia¹; ¹Penn Epigenetics Institute, Dept. of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; ²Dept. of Medicine, Division of Gastroenterology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- MOB am 09:30 **Metabolic Tracing in Hepatocytes Demonstrates the Contribution of acetyl-CoA Derived from Ethanol Metabolism to Histone Acetylation;** Crystina Kriss¹; Stanley M Stevens Jr²; ¹University of South Florida, Tampa, FL; ²University of South Florida, Tampa, FL
- MOB am 09:50 **Quantitative *in vitro* Proteomic Profiling of Colon Cancer Spheroids treated with Combination Chemotherapy in a 3D printed Fluidic Device;** Gabriel LaBonia¹; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN
- MOB am 10:10 **Resolution of ^{13}C and Deuterium Isotopes Allows Lipid Fluxomics Analysis By Rate of Deuterium Incorporation;** Matthew Mitsche¹; Goncalo Vale¹; Jeffrey McDonald¹; ¹University of Texas Southwestern Medical Center, Dallas, TX

8:30-10:30 am Monday

METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS

Leah Shriver (University of Akron)

Sagamore 1-3 level 2

- MOC am 08:30 **A Metabo-Redoxome Platform for Comprehensive Survey of Oxidative Stress Severity in the Lower Respiratory Tract of Smokers and HIV-infected Subjects;** Miriam Sindelar¹; Sarah L O'Beirne¹; Philip L Leopold¹; Michelle R Staudt¹; Robert J Kaner¹; Ronald G Crystal¹; Steven S Gross¹; ¹Weill Cornell Medicine, New York, NY
- MOC am 08:50 **Stable Isotope-Resolved Metabolomic (SIRM) Studies of *in vitro*, *in vivo*, and *ex vivo* Isogenic Human Cancer Models Using Ion-Chromatography MS;** Marc O. Warmoes¹; Qiushi Sun¹; Ramon Sun¹; Penghui Lin¹; Andrew N. Lane¹; Richard M. Higashi¹; Teresa W.-M. Fan¹; ¹University of Kentucky, Lexington, KY
- MOC am 09:10 **Differentiation of Acylcarnitine Isomers Based on LC-MS/MS Mass Spectra and Development of an Accurate Mass Spectral Library;** Xinjian Yan¹; Yuri Mirokhin¹; Ramesh Marupaka¹; Yamil Simón-Manso¹; Dmitrii Tchekhovskoi¹; Stephen E Stein¹; ¹NIST, Gaithersburg, MD
- MOC am 09:30 **Microprobe Single-cell CE-ESI-MS Captures Metabolic Changes in the Developing Frog (*Xenopus laevis*) Embryo;** Rosemary Masu Onjiko¹;

MOC am 09:50

MOC am 10:10

Erika P Portero¹; Sally A Moody¹; Peter Nemes¹; ¹George Washington University, Washington, DC

Solid Phase Microextraction: A New Tool for *in vivo* monitoring of Metabolic Changes Occurring During Deep Brain Stimulation; Nathaly Reyes Garces¹; Ezel Boyaci¹; German A. Gomez-Rios¹; Barbara Bojko^{1,2}; Clement Hamani³; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON, Canada; ²Nicolaus Copernicus University in Torun, Bydgoszcz, Poland; ³University of Toronto, Toronto, ON, Canada

FAC-MS: A New Platform Coupling Heterologous Expression and Untargeted Metabolomics for Large-Scale Fungal Natural Product Discovery; Ken Clevenger¹; Jinwoo Bok²; Rosa Ye³; Galen P Miley⁴; Maria H Verdan⁴; Thomas Velk²; Cynthia Chen³; KaHoua Yang²; Matthew Robey⁴; Peng Gao⁴; Matthew Lamprecht³; Md Nurul Islam³; Jonathan Palmer⁵; PAUL Thomas⁴; ChengCang Wu³; Nancy Keller²; Neil L Kelleher⁴; ¹Northwestern University, Evanston, IL; ²University of Wisconsin Madison, Madison, WI; ³Intact Genomics, St. Louis, MO; ⁴Northwestern University, Evanston, IL; ⁵US Forest Service, Madison, WI

8:30-10:30 am Monday

INNOVATIONS AND APPLICATIONS IN FORENSICS

Marilyn Tourne (Tuskegee University)

Sagamore 4 level 2

- MOD am 08:30 **Paper Spray Mass Spectrometry for the Detection of Chemical Warfare Agent Simulants;** Elizabeth S Dhumakupt^{1,2}; Josiah McKenna³; Theresa Connell⁴; Paul Demond⁴; Dennis B Miller¹; Nicholas E Manicke³; J Michael Nilles⁴; Trevor Glaros¹; ¹US Army ECBC, Aberdeen Proving Ground, MD; ²National Research Council, Washington, DC; ³Indiana University-Purdue University Indianapolis, Indianapolis, IN; ⁴Excet, Inc., Springfield, VA
- MOD am 08:50 **Development of a High Sensitivity Method for Direct Characterisation of Forensic Samples;** Efstathios Elia¹; Samantha Leach²; I-Chung Lu¹; Milan Pophristic³; Sarah Trimpin¹; ¹Wayne State University, Detroit, MI; ²DC Department of Forensic Sciences (DFS), Washington, DC; ³MSTM, LLC., Newark, DE
- MOD am 09:10 **Rapid Absolute Quantification of Abrin Toxin and Its Isoforms in Complex Matrices by Immuno-extraction and High Resolution Targeted Mass Spectrometry;** Eva-Maria Hansbauer¹; Sylvia Worbs²; François Fenaille¹; Hervé Volland³; Stéphanie Simon³; Christophe Junot¹; Brigitte G. Dorner²; François Becher¹; ¹CEA Saclay, DRF, iBiTec-S, Service de Pharmacologie et d'Immunoanalyse, Laboratoire d'Etude du Métabolisme des Médicaments, Gif-sur-Yvette, France; ²Biological Toxins, Centre for Biological Threats and Special Pathogens, Robert Koch Institute, Berlin, Germany; ³CEA Saclay, DRF, iBiTec-S, Service de Pharmacologie et d'Immunoanalyse, Laboratoire d'Etudes et de Recherches en Immunoanalyse, Gif-sur-Yvette, France
- MOD am 09:30 **Identification of Fentanyl and Other Synthetic Opiates using Ambient Ionization High Resolution Time-of-Flight Mass Spectrometry;** Jamie Foss¹; Amanda Moore²; Sabra Botch-Jones²; Maria Pease³; Frank Kero⁴; ¹PerkinElmer, Shelton, CT; ²Boston University School of Medicine, Boston, MA; ³Maine Health and Environmental Testing Laboratory, Augusta, ME; ⁴PerkinElmer, Downers Grove, IL



MOD am 09:50 **Development of Solid Phase Microextraction (SPME) Devices for Analysis of Drugs in Biofluids via Direct Analysis in Real Time (DART)**; Tijana Vasiljevic¹; German Augusto Gomez-Rios¹; Emanuela Gionfriddo¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON, Canada

MOD am 10:10 **Isomeric Separation of Cannabinoids by UPLC-ESI(±)TWIM-MS**; Lilian V. Tose¹; Samantha R.C. Silva¹; Michael Murgu²; Boniek Gontijo Vaz^{3,4}; Wanderson Romão^{4,5}; ¹Federal University of Espírito Santo, Vitória, Brazil; ²Waters Corporation, São Paulo, Brazil; ³Federal University of Goiás, Goiânia, GO; ⁴National Institute of Forensic Science and Technology (INCT), Vila Velha, Brazil; ⁵IFES/UFES, Vila Velha, Brazil

8:30-10:30 am Monday

PLANT "OMICS"

Erin Gemperline (Dow Agrosciences)

Sagamore 5-7 level 2

MOE am 08:30 **Plant Ionomics Profiling: Development of a High-throughput Multi-elemental Profiling Technique Using ICP-MS and Case Studies in Onion, Potato and Barley**; Jacqueline M. Chaparro^{1,2}; Corey D. Broeckling¹; Jessica E. Prenni¹; Adam L. Heuberger²; ¹Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; ²Colorado State University Department of Horticulture and Landscape Architecture, Fort Collins, CO

MOE am 08:50 **Direct Identification of Mosaic Virus Induced Molecular Signature Changes in Plant Leaves Using High Throughput Laser-REIMS Technology**; Richard Schäffer¹; Julia Balog^{2,3}; Gabriel Horkovics-Kovats²; Tamas Karancsi²; Steven Derek Pringle^{3,4}; Katalin Salánki⁵; Ákos Gellért⁵; Zoltan Takats³; ¹Waters Research Center, Budapest; ²Waters Research Center, Budapest; ³Imperial College London, London; ⁴Waters Corporation, Wilmslow, UK; ⁵Centre for Agricultural Research, Hungarian Academy of Sciences, Budapest, Hungary

MOE am 09:10 **Implementation of a Spatial Metabolomics Approach for Exploring Interactions within a Tripartite Plant-Fungus-cyanobacterium System**; Dusan Velickovic¹; Alyssa A. Carrell²; Rosalie K. Chu¹; Malak M. Tfaily¹; Dale Pelletier³; Samuel M. D. Seaver⁴; Mathew Thomas¹; Ljiljana Pasa-Tolic¹; David J. Weston^{2,3}; Christopher R. Anderson¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Department of Biology, Duke University, Durham, NC; ³Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; ⁴Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL

MOE am 09:30 **Proteomic Profiling to Identify the Unintended Effects of Genetic Modification on Gluten Proteins**; Sophie Bromilow¹; Lee A. Gethings²; Mike Buckley³; Peter Shewry⁴; E. N. C. Mills¹; ¹School of Biological Science, Manchester Institute of Biotechnology, Manchester, UK; ²Waters Corporation, Wilmslow, UK; ³School of Environmental Sciences, Manchester Institute of Biotechnology, Manchester, UK; ⁴Rothamsted Research, Harpenden, UK

MOE am 09:50 **Large Scale Integration of Proteomics and Genomics Data to Enhance Rice Genome Annotation**; Da Qi¹; Zhe Ren²; Bo Wen²; Ruo Zhou²; Siqi Liu^{2,3}; Andrew R. Jones¹; ¹University of Liverpool, Liverpool, UK; ²The BGI-Shenzhen, Shenzhen, China; ³Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China

MOE am 10:10 **Streamlining Phosphoproteomic Workflow to Study Plant Signaling and Its Application to Tomato Phosphoproteomics**; Chuan-Chih Hsu¹; Yingfang Zhu¹; Pengcheng Wang¹; Peipei Zhu¹; I-Hsuan Chen¹; Yuan Zhou¹; Jian-Kang Zhu¹; Andy Tao¹; ¹Purdue University, West Lafayette, IN

8:30-10:30 am Monday

ION MOBILITY: NEW DEVELOPMENTS & APPLICATIONS

Theresa Evans-Nguyen (Univ. of Southern Florida)

Wabash level 1

MOF am 08:30 **A New Instrument with High Mass and High Ion Mobility Resolution**; Michael T. Bowers¹; Thomas Wytenbach²; Paul R. Kemper²; Mel Park³; Goekhan Baykut⁴; ¹University of California, Santa Barbara, CA; ²University of California Santa Barbara, Santa Barbara, CA; ³Bruker Daltonics, Billerica, MA; ⁴Bruker Daltonik GmbH, Bremen, Germany

MOF am 08:50 **Discovery and Targeted Monitoring of D. discoideum Lipids using Multidimensional LC-TIMS-MS/MS Separations**; Kendra J. Adams¹; Cesar E. Ramirez¹; Richard H. Gomer²; Francisco Fernandez-Lima^{1,3}; ¹Florida International University, Miami, FL; ²Texas A&M University, College Station, Texas; ³Biomolecular Sciences Institute, Miami, FL

MOF am 09:10 **Conformationally Dependent Peptide Hydrolysis Measured by Temperature Controlled ESI-IMS-MS**; Daniel R. Fuller¹; Christopher R. Conant¹; Tarick J. El-Baba²; Zhichao Zhang²; Daniel W. Woodall²; David H. Russell³; David E. Clemmer²; ¹Indiana University Bloomington, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN; ³Texas A&M University, College Station, TX

MOF am 09:30 **Multidimensional, Time-resolved Trapped Ion Mobility Spectrometry-Mass Spectrometry (TIMS/TIMS-MS) to Elucidate Conformations of Proteins**; Fanny Caroline Liu¹; Mark E. Ridgeway²; Melvin A. Park²; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL; ²Bruker Daltonics, Billerica, MA

MOF am 09:50 **Transformational Approaches for Realizing High Resolution, High Throughput Ion Mobility Measurements: Compressive Sensing and Ion Multiplexing**; Austen L. Davis¹; Brian H. Clowers¹; ¹Washington State University, Pullman, WA

MOF am 10:10 **Exploring Rigidity and Flexibility with Ion Mobility Mass Spectrometry: From Synthetic Knots to Disordered Proteins**; Rachelle Black¹; Lukasz Migas¹; Eleanor Dickinson¹; Bruno Bellina¹; Kamila J. Pacholarz¹; Perdita E. Barran²; ¹The University of Manchester, Manchester, UK; ²The University of Manchester, Manchester, Greater Manchester

8:30-10:30 am Monday

INSTRUMENTATION: NEW DEVELOPMENTS IN ION DETECTION

Mark Bier (Carnegie Mellon University)

Room 101-106 level 1

MOG am 08:30 **Mass and Stiffness Spectrometry based on 2D Scanning Multimode Nanomechanical Resonators for Biological Applications**; Oscar Malvar¹; Jose Jaime Ruz¹; Priscila Monteiro Kosaka¹; Carmen Martínez Domínguez¹; Eduardo Gil-Santos¹; Dimitris Papanastasiou²; Monsterrat Calleja¹; Javier Tamayo¹; ¹CSIC, Tres Cantos, Madrid; ²Fasmatech Science & Technology, Athens, Greece

MOG am 08:50 **Decreasing Uncertainty in the Mass-to-Charge Measurement in Charge Detection Mass Spectrometry with an Improved Ion Trap and Detector**; Joanna Hogan¹; Martin Jarrold²; ¹Indiana



MONDAY MORNING ORAL SESSIONS

- MOG am 09:10 *University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN*
High Resolution Stigmatic Ion Imaging of Single Cells using a Timepix Pixel Detector; Anne L. Bruinen¹; Rachel Balez²; Nino Iakobachvili¹; Joel Keelor¹; Shane R. Ellis¹; Ron MA Heeren¹; ¹M4I Institute - Maastricht University, Maastricht, Netherlands; ²Illawarra Health and Medical Research Institute, School of Biological Sciences, University of Wollongong, Wollongong, Australia
- MOG am 09:30 **Development of High Intensity Biomolecular ion Beam with Quantitative and Qualitative Measurement;** Szu-Hsueh Lai^{1,2}; Jung-Lee Lin¹; Chung-Hsuan Chen^{1,2}; ¹Genomics Research Center Academia Sinica, Taipei; ²National Taiwan University, Taipei, Taiwan
- MOG am 09:50 **High-Resolution Helium and Argon Isotope Analysis by Ion Counting in a Small, Multi-Turn Time-of-Flight Mass Spectrometer;** Kirk Richard Jensen¹; Toshinobu Hondo^{1,2}; Yosuke Kawai³; Hirochika Sumino⁴; Michisato Toyoda¹; ¹Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Toyonaka, Japan; ²MS-Cheminformatics, LLC, Inabe-gun, Japan; ³Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Japan; ⁴3. Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Meguro-ku, Japan
- MOG am 10:10 **Novel Data Acquisition Approaches for Enhanced Ion Detection in FTMS Instruments;** Anton N. Kozhinov¹; Konstantin O. Nagornov¹; Yuri O. Tsybin¹; ¹Spectroswiss Sàrl, Lausanne, Switzerland

8:30-10:30 am Monday
SYNTHETIC POLYMERS
Chrys Wesdemiotis (University of Akron)
Room 107-110 level 1

- MOH am 08:30 **Characterization of Synthetic Fibers and their Finish Layer by LAESI - MS;** Freddie van Geenen^{1,2}; Maurice Franssen¹; Han Zuilhof¹; Michel Nielsen^{1,3}; ¹Wageningen University, Wageningen, Netherlands; ²TI-Coast, Amsterdam, Netherlands; ³RIKILT Wageningen University & Research, Wageningen, Netherlands

- MOH am 08:50 **Paper Spray and Kendrick Mass Defect Analysis of Block and Random Copolymers;** Robert B. Cody¹; Thierry Fouquet²; Kanae Teramoto³; Koji Okuda⁴; Andrew John Dane⁴; Evgeny Tishchenko⁴; ¹JEOL USA, Inc., Peabody, MA; ²National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; ³JEOL Ltd., Akishima, Japan; ⁴JEOL USA Inc., Peabody, MA
- MOH am 09:10 **Improving the Resolution of the Kendrick Mass Defect Analysis of Polymer Ions with Fractional Base Units;** Thierry Fouquet¹; Hiroaki Sato¹; ¹National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan
- MOH am 09:30 **Full Hydrogen/Alkali Exchange in Positive Mode Electrospray Ionization to Simplify MS/MS Reading of Information Digitally Encoded in Sequence-defined Polyurethanes;** Salomé Poyer¹; Jean-Arthur Amalian¹; Benoit Eric Petit²; Sophia Telitel²; Denise Karamessini²; Jean-François Lutz²; Laurence Charles¹; ¹Aix-Marseille University, Marseille, France; ²Institut Charles Sadron, CNRS, Strasbourg, France
- MOH am 09:50 **Materials Compatibility Study: 3D Printer Materials;** James D Wright Jr¹; Mary Margaret Wade¹; Bradley Ruprecht¹; Richard Moore¹; Jonathan Oyler²; Kelly Smith²; ¹US Army ECBC, APG, MD; ²USARMY MEDCOM USAMRICD, APG, MD
- MOH am 10:10 **Thermally-Induced Reaction Mechanisms of Benzocyclobutene-Based Polymers;** Anthony Paul Gies¹; Nathan J. Rau¹; Liam Spencer¹; ¹The Dow Chemical Company, Freeport, TX

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.

MONDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Monday
MS IN CLINICAL ANALYSIS
Julie Ray (ARUP)
Hall D level 1

- MOA pm 02:30 **Development and Validation of a Sensitive LC-MS/MS Method for Analysis of Milrinone in Pediatric Plasma;** Ganesh Moorthy¹; Annie Giaccone¹; Athena F Zuppa¹; ¹The Children's Hospital of Philadelphia, Philadelphia, PA
- MOA pm 02:50 **A Fast Method for the Detection of Antiepileptic Drugs in Human Urine Using Positive-Negative Polarity Switching LC-MS/MS;** Brandi R. Bridgewater¹; Erin C. Strickland²; Gregory L. McIntire²; ¹Ameritox, LLC, Greensboro, NC; ²Ameritox, LLC, Greensboro, NC
- MOA pm 03:10 **Accurate Quantitation and Stability Testing of 21 Amino Acids on Dried Blood Spots by UPLC/MS/MS;** Jun Han¹; Rehan Higgins¹; Juncong Yang¹; Karen Lin¹; Christoph H. Borchers^{1,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochemistry

and Microbiology, University of Victoria, Victoria, BC, Canada

- MOA pm 03:30 **More (Sensitivity) is Always Better: Measuring Sub-clinical Levels of Thyroglobulin in Human Serum on a Micro-flow LC-MS/MS System;** Christopher M. Shuford¹; Jay S. Johnson²; J. Will Thompson³; Patricia L. Holland¹; James Murphy²; Russell P. Grant¹; ¹Laboratory Corporation of America, Burlington, NC; ²Waters Corp, Milford, MA; ³Duke University, Durham, NC
- MOA pm 03:50 **A Highly Sensitive LC-MS/MS Method for the Simultaneous Quantitation of 3 α and 3 β Androstane-3,17 β Diol in Post-Menopausal Serum;** Yuyong Ke¹; Alain Dury¹; Renaud Gonthier¹; Fernand Labrie¹; ¹EndoCeutics, Quebec, QC, Canada
- MOA pm 04:10 **Determination of 25-hydroxyvitamin D in Aqueous Cellular Environments by LC-MS/MS Using the Novel Chemical Derivatization Reagent MDBP;** Miriam J. Mueller¹; Dietrich A. Volmer¹; ¹Saarland University, Saarbruecken, Germany



2:30-4:30 pm Monday
ANALYTICAL CHALLENGES OF MICRODOSING AND
MICROSAMPLING STUDIES
Lucinda Hittle (Merck & Co)
500 Ballroom level 1

- MOB pm 02:30 **Development of Small Sample Volume Methods to Measure Drugs in Pediatric Patients: Moving Toward One-drop Blood Assays;** Liusheng Huang¹; Janel Long-boyle²; Francesca Aweeka²; ¹San Francisco General Hospital, UCSF, San Francisco, CA; ²UCSF, San Francisco, CA
- MOB pm 02:50 **Dried Blood Spots in Tips Targeted Drug Screening in 9 Seconds per Sample Using Laser-Diode-Thermal-Desorption Mass Spectrometry (LDTD-MS/MS);** Jonathan Rochon¹; Pier-Luc Plante²; Serge Auger³; Jacques Corbeil²; Réal Paquin²; Jean Lacoursiere³; Pierre Picard³; ¹Université Laval, Québec, QC, Canada; ²Université Laval, Québec, Québec; ³Phytronix Technologies, Québec, QC, Canada
- MOB pm 03:10 **Testing Anabolic Agents from Exhaled Breath for Doping Control Purposes Using Liquid Chromatography / High- and Low-resolution Tandem Mass Spectrometry;** Mario Thevis^{1,2}; Oliver Krug^{2,3}; Hans Geyer^{2,3}; Andreas Thomas³; Thomas Piper³; Josef Dib³; Andreas Lagojda⁴; Dirk Kuehne⁴; Wilhem Schänzer³; ¹German Sport University, Cologne, NRW; ²European Monitoring Center for Emerging Doping Agents, Cologne/Bonn, Germany; ³German Sport University Cologne, Cologne, Germany; ⁴Bayer AG, Monheim, Germany
- MOB pm 03:30 **Comprehensive Glycomic and Proteomic Profiling from Histopathological Sections of Breast Cancers: A Comparison Study of Tumor Heterogeneity;** Le Meng¹; Nicolas Bloch²; Robert Pistey²; Joshua A. Klein²; Joseph Zaia²; ¹Boston University School of Medicine, Boston, MA; ²Boston University School of Medicine, Boston, MA
- MOB pm 03:50 **Mass Spectrometry Profiling of *in vitro* Tumors Using the Single-probe Device;** Xiang Tian¹; Wei Rao¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK
- MOB pm 04:10 **Development of Chemical Isotope Labeling Nanoflow LC-MS for High-Coverage Metabolomic Profiling of 100 to 1000 Cancer Cells;** Xian Luo¹; Liang Li¹; ¹University of Alberta, Edmonton, Alberta

2:30-4:30 pm Monday
METABOLOMICS: UNTARGETED PROFILING
Andrew Patterson (Penn State University)
Sagamore 1-3 level 2

- MOC pm 02:30 **Annotation of Challenging Signals in Untargeted Metabolomics;** Nathaniel G Mahieu¹; Gary J Patti²; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University in St. Louis, St. Louis, MO
- MOC pm 02:50 **Increasing Compound Identification Rates in Untargeted Metabolomics Research;** Ivana Blaženović¹; Tobias Kind¹; Hrvoje Torbašinović²; Slobodan Obrenović²; Sajjan S. Mehta¹; Oliver Fiehn¹; ¹Metabolomics Fiehn Lab, Genome Center, University of California, Davis, California; ²Inovatus, Zagreb, Croatia
- MOC pm 03:10 **Curated Open-access LC-Orbitrap-MS/MS Spectral Library of Endogenous Metabolites and Lipids;** Prasad Phapale; Andrew Palmer; Dominik Fay; Ivan Protsyuk; Theodore Alexandrov; EMBL, Heidelberg, Germany
- MOC pm 03:30 **Extending a Comprehensive Reference Tandem Mass Spectral Library for More Reliable Metabolite Identification;** Xiaoyu Yang¹; Pedatsur

- MOC pm 03:50 **Purification, Concentration and Metabolite Identification of Endogenous Urine Metabolites in Large Scale Phenotyping Studies;** Luke Whitley¹; Elena Chekmeneva²; David J Berry¹; Zoltan Takats²; Elaine Holmes²; Jeremy K Nicholson^{1,2}; Matthew Lewis¹; ¹MRC-NIHR National Phenome Centre, Imperial College London, London, UK; ²Division of Computational and Systems Medicine, Department of Surgery and Cancer, Imperial College London, London, UK
- MOC pm 04:10 **Untargeted Metabolomics of 2400 American Gut Project Participants Reveals Information About Our Health, Behavior, and Microbiota;** Alan K. Jarmusch¹; Embriette R Hyde²; Alexey V. Melnik¹; Alexander Aksenov¹; Daniel McDonald²; Ricardo da Silva¹; Lindsay DeRight-Goldasich²; Paul Wischmeyer³; Rob Knight²; Pieter C. Dorrestein¹; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ²Department of Pediatrics, University of California San Diego, La Jolla, CA; ³Duke University School of Medicine, Durham, NC

2:30-4:30 pm Monday
ENVIRONMENTAL: EMERGING CONTAMINANTS
Paul Chiarelli (Loyola University Chicago)
Sagamore 4 level 2

- MOC pm 02:30 **Combining Non-Target and Target Screening of DBPs: Assessing Removal Strategies to Make Drinking Water Safer;** Susan Richardson¹; Amy A. Cuthbertson¹; Susana Y. Kimura¹; Hannah K. Liberatore¹; Detlef Knappe²; Benjamin Stanford³; R. Scott Summers⁴; Eric Dickenson⁵; Chad Seidel⁶; Clark Maness²; Riley Mulhern⁴; Amlan Ghosh⁶; Jonathan D Byer⁷; ¹University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; ²North Carolina State University, Raleigh, NC; ³Hazen and Sawyer, Raleigh, NC; ⁴University of Colorado, Boulder, CO; ⁵Southern Nevada Water Authority, Las Vegas, NV; ⁶Corona Environmental Consulting, Boulder, CO; ⁷LECO Corporation, Saint Joseph, MI
- MOC pm 02:50 **Organic Pollutants in the Clouds of the Center of France;** Olga Polyakova¹; Viatcheslav Artaev²; Isabelle Canet³; Audrey Lallement³; Pierre Amato³; Mickael Vaitilingom^{3,4}; Anne-Marie Delort³; Albert T. Lebedev¹; ¹Moscow State University, Moscow, Russia; ²LECO Corporation, Saint Joseph, MI; ³Clermont Université Auvergne, CNRS, Sigma-Clermont, Institut de Chimie de Clermont-Ferrand, F-63000, Clermont-Ferrand, France; ⁴Clermont Université Auvergne, CNRS, LaMP/OPGC, F-63000, Clermont-Ferrand, France
- MOD pm 03:10 **Potential Environmental Effects of Unconventional Oil and Gas Extraction: A Menu of New Mass Spectrometry Methods for Advanced Monitoring;** Doug D. Carlton^{1,2}; Zacariah L. Hildenbrand^{2,3}; Ines C. Santos¹; Kevin A. Schug^{1,2}; ¹The University of Texas at Arlington, Arlington, TX; ²Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, Texas; ³Inform Environmental, LLC, Dallas, Texas
- MOD pm 03:30 **Kendrick Mass Defect Analysis in Environmental Non-target Screening: Identification of Ozonation By-products in Water Treatment;** Sylvain Merel¹; Sascha Lege¹; Christian Zwiener¹; ¹Universität Tübingen, Tübingen, Germany



MONDAY AFTERNOON ORAL SESSIONS

- MOD pm 03:50 **Identification of Disperse Dyes in House Dust: A Novel Class of Emerging Indoor Contaminants Relevant to Human Exposure**; Lee Ferguson¹; Heather M Stapleton²; ¹Duke University, Durham, NC; ²Duke University, Durham, NC
- MOD pm 04:10 **Determination of Nitro-Musks in Wastewater Using QuEChERS Method Combined with Electron Capture Negative Ion GC/Tandem Mass Spectrometry**; Tommy Bisbicos¹; Grazina Pacepavicius¹; Mehran Alaei¹; ¹Environment and Climate Change Canada, Burlington, ON, Canada

2:30-4:30 pm Monday HYDROGEN-DEUTERIUM EXCHANGE MS Claudia Maier (Oregon State University) Sagamore 5-7 level 2

- MOE pm 02:30 **Probing the Intracellular Structure of α -synuclein by In-Cell Hydrogen/Deuterium Exchange**; Jeppe Buur Madsen¹; Cagla Sahin^{2,3}; Daniel Otzen^{2,3}; Poul Henning Jensen⁴; Thomas J.D. Jørgensen¹; ¹University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense M, Denmark; ²Aarhus University, Interdisciplinary Nanoscience Center, Aarhus C, Denmark; ³Aarhus University, Department of Molecular Biology and Genetics, Aarhus C, Denmark; ⁴Aarhus University, DANDRITE—Danish Research Institute of Translational Neuroscience & Department of Biomedicine, Aarhus C, Denmark
- MOE pm 02:50 **Analyzing Histone Dynamics Using Hydrogen-Deuterium Exchange coupled to Top-down and Middle-down Mass Spectrometry**; Kelly Karch; Mariel Coradin; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- MOE pm 03:10 **Top-down HDX Analysis of Proteins Using Ultraviolet Photodissociation**; Nicholas I. Brodie¹; Evgeniy V. Petrotchenko¹; Jingxi Pan¹; Terry Zhang²; Romain Huguet²; Rosa Viner²; Vlad Zabrouskov²; Christoph H. Borchers^{3,4}; ¹University of Victoria-Genome British Columbia Proteomics Centre, Victoria, BC, Canada; ²Thermo Fisher Scientific, San Jose, CA; ³University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ⁴Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MOE pm 03:30 **Probing Protein Structure via Surface Induced Dissociation and Gas Phase Hydrogen-Deuterium Exchange in a Hybrid FT-ICR**; Jing Yan¹; Arpad Somogyi¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- MOE pm 03:50 **Identification of Epitopes in Japanese Encephalitis Virus Envelope Protein and Characterization of Antigen Antibody Complexes by Mass Spectrometry**; Jagat Adhikari¹; Melissa A. Edeling²; James Heffernan²; Estefania Fernandez²; Michael S. Diamond²; Daved H. Fremont²; Michael L. Gross¹; ¹Washington University, St Louis, MO; ²Washington University School of Medicine, St Louis, MO
- MOE pm 04:10 **Hydrogen-Deuterium Exchange MS Provides Insights into Structural Dynamics of Apolipoprotein A-I and its Disease-causing Mutants on Model Discoidal High-density Lipoproteins**; Christopher Wilson¹; Madhurima Das²; Xiaohu Mei²; Olga Gursky²; John R Engen¹; ¹Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; ²Department of Physiology and Biophysics, Boston University School of Medicine, Boston, MA

2:30-4:30 pm Monday ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS, AND DMPK Kimberly Kew (East Carolina University) Wabash level 1

- MOF pm 02:30 **Utilising Ion-mobility Mass Spectrometry and Molecular Modelling to Screen for Synthetic Biology Targets**; Eleanor Sinclair¹; Cunyu Yan¹; Maria Vinaixa¹; Perdita E Barran¹; ¹University of Manchester, Manchester, UK
- MOF pm 02:50 **Matrix-Assisted Ionization - Ion Mobility Spectrometry - Mass Spectrometry for the Characterization of Drugs Directly from Biological or Synthetic Environments**; Ellen D. Inutan^{1,2}; Trine G. Halvorsen³; Wen-Jing Zhang¹; I-Chung Lu¹; James Wager-Miller⁴; Srinivas B. Narayan⁵; David Crich¹; Ken Mackie⁴; SARAH TRIMPIN^{1,2}; ¹Department of Chemistry, Wayne State University, Detroit, MI; ²MSTM, LLC, Newark, DE; ³Dept. Pharmaceutical chemistry School of Pharmacy University of Oslo, Oslo, Norway; ⁴Psychology and Brain Sciences, Indiana University, Bloomington, IN; ⁵Detroit Medical Center University Laboratories - Core, Detroit, MI
- MOF pm 03:10 **Determination of pH-induced Oligomerization of a Lipidated Peptide by IMS-MS**; Elizabeth E. Pierson¹; Nicholas A Pierson¹; ¹Merck Research Laboratories, Rahway, NJ
- MOF pm 03:30 **Quantitation of Urinary Acetylcarnitine in Radiation Exposed Non-Human Primates (NHP) is Dependent upon the Calibration Curve Matrix**; Nicholas B. Vera^{1,2}; Evan Pannkuk³; Evagelia C. Laiakis⁴; A.J. Fornace, Jr.⁴; Stephen L. Coy²; Derek M. Erion¹; Paul Vouras²; ¹Pfizer, Cambridge, MA; ²Northeastern University, Boston, MA; ³Tumor Biology Program, Lombardi Comprehensive Cancer Center, Georgetown University, Washington, DC; ⁴Georgetown University, Washington, DC
- MOF pm 03:50 **Differential Mobility – Mass Spectrometry Metabolomics Platform for Biomarker Discovery in Chronic Kidney Disease**; Stefanie Wernisch¹; Thekkelnaycke Rajendiran¹; Subramaniam Pennathur¹; ¹University of Michigan, Ann Arbor, MI
- MOF pm 04:10 **Comparison of the Selected Metal Binding Characteristics of the Methanobactin from *Methylosinus trichosporium* OB3b**; Laurence Angel¹; Jacob W McCabe¹; Rajpal Vangala¹; ¹Texas A&M University - Commerce, Commerce, TX

2:30-4:30 pm Monday INSTRUMENTATION: AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS Mari Prieto (Thermo Scientific) Room 101-106 level 1

- MOG pm 02:30 **Novel Simplified Data Mining Approach Facilitates Rapid Fingerprinting of Lignin via Ambient Ionization High-resolution Mass Spectrometry**; Elizabeth A. Crawford¹; Stefanie Gerbig²; Bernhard Spengler²; Dietrich A. Volmer¹; ¹Saarland University, Saarbruecken, Germany; ²Justus Liebig University Giessen, Giessen, Germany
- MOG pm 02:50 **Paper Spray Chemical Ionization for the Detection of Femtomole Levels of Non-polar to Less Polar Compounds**; Donghui Kim¹; Un Hyuk Yim²; Byungjoo Kim³; Sangwon Cha⁴; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, South Korea; ²Korea Institute of Ocean Science and Technology, Geoje, South Korea; ³Korea Research Institute of Standards and Science, Daejeon, South Korea; ⁴Hankuk University of Foreign Studies, Yongin, South Korea



- MOG pm 03:10 **Delayed Desorption Improves Protein Analysis by Desorption Electrospray Ionization Mass Spectrometry**; Tara L. Maser¹; Elahe Honarvar¹; Andre R. Venter¹; ¹Department of Chemistry, Western Michigan University, Kalamazoo, MI
- MOG pm 03:30 **Transmission Low Temperature Plasma Probe for *in situ* Mass Spectrometry Analysis with Paper Analytical Devices**; Yaoyao Zhao¹; Xiaoxiao Ma²; Zhenwei Wei¹; Hansen Zhao¹; Jia Jia¹; Sichun Zhang¹; Zheng Ouyang^{1,2}; Xinrong Zhang¹; ¹Tsinghua University, Beijing, Beijing; ²Purdue, West Lafayette, IN
- MOG pm 03:50 **Coupling of a Versatile Three-Electrode Paper-Based Electrochemical Cell to Mass Spectrometry: Electrochemical Sonic Spray Ionization Mass Spectrometry**; Yao-Min Liu¹; Yeyoung Ha¹; Andrew A. Gewirth¹; ¹University of Illinois at Urbana Champaign, Urbana, IL
- MOG pm 04:10 **Triboelectric Nanogenerators (TEGs) for Nano-Coulomb Ionization Mass Spectrometry**; Anyin Li¹; Yunlong Zi²; Zhong Lin Wang²; Eacundo M Fernandez²; ¹Georgia Institute of Technology, Atlanta, GA; ²Georgia Institute of Technology, Atlanta, GA

2:30-4:30 pm Monday

FUNDAMENTALS: ION-ION AND ION-NEUTRAL INTERACTIONS
Scott McLuckey (Purdue University)
Room 107-110 level 1

- MOH pm 02:30 **Charge Transfer Dissociation (CTD): High Energy Radical Fragmentation of Glycans, Proteins and Peptides**; Glen Paul Jackson¹; Pengfei Li²; David Ropartz³; Helene Rognaux⁴; ¹West Virginia University, Morgantown, WV; ²West Virginia University, Morgantown, WV; ³INRA, UR1268 Biopolymers Interactions Assemblies, Nantes, France; ⁴INRA, UAR1008, Nantes, France
- MOH pm 02:50 **Gas-Phase Peptide Bioconjugation with PLP and the Identification of Activation Site by Accumulative Tandem Mass Spectrometry**; Muyi HE¹; You Jiang²; Sijian Ye³; Xiang Fang²; Wei Xu¹;

- ¹Beijing Institute of Technology, Beijing, Beijing;
²National Institute of Metrology, Beijing, China;
³Changchun University of Science and Technology, Changchun, China
- MOH pm 03:10 **Studying Reduced Metal Complexes via Sequentially Coupled Ion/Ion-Ion/Molecule Reactions**; Mariah Parker¹; Scott Gronert²; ¹Virginia Commonwealth University, Richmond, VA; ²Virginia Commonwealth University, Richmond, Virginia
- MOH pm 03:30 **Dual Cryogenic Ion Trap Spectrometer for Temperature-controlled Ion-molecule Reactions and Clustering**; Etienne Garand¹; Erin M Duffy²; Jonathan M Voss²; Kaitlyn Fischer²; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin-Madison, Madison, WI
- MOH pm 03:50 **Gas-phase Peptide Cross Linking for Probing the Nature of Non-covalent Bonding of a Peptide Related to Brain Damage**; Yang Liu¹; Emilie Viglino¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA
- MOH pm 04:10 **Differentiating N- Versus O-Glucuronide Metabolites via Ion/Molecule Reactions**; John Kong¹; Zaikuan Yu¹; Edouard Niyonsaba¹; Ravikiran Yerabolu¹; Xin Ma¹; McKay Easton¹; Duanchen Ding¹; Hanyu Zhu¹; Huaming Sheng²; Tiffany Jarrell²; Zhoupeng Zhang²; Hilkka Kenttamaa¹; ¹Purdue University, West Lafayette, IN; ²Merck & Co., Inc, Kenilworth, NJ

4:45-5:30 pm Monday

AWARD LECTURE
Vicki Wysocki (The Ohio State University)
Hall D level 1



Award for a Distinguished Contribution in Mass Spectrometry

Catherine E. Costello
Boston University

5:45 - 7:00 PM MONDAY WORKSHOPS

There are light refreshments in common areas.

01. Improving Scientific Writing Skills
Presiding: Christopher Petucci
Room 130

"The difference between the almost right word and the right word is really a large matter - it's the difference between the lightning bug and the lightning (Mark Twain)." The ability to write grammatically correct sentences and succinct paragraphs is essential to clearly communicate ideas. This workshop will be a hands-on session for logical, clear paragraph development. Specific topics include essential grammar for scientific writing, writing grammatically correct sentences, and clearly organizing and developing your ideas in written form. At the conclusion of this session, you will have an increased knowledge of the basic writing skills to prepare manuscripts with greater clarity for theses, grant submissions, and scientific journals.

Would this workshop be of interest to the Undergraduate Research in MS and Young Mass Spectrometrists interest groups?

02. Metal Ion Coordination in Gas-Phase Bioanalysis: Reaping Practical Benefits
(Metal Ion Coordination Chemistry Interest Group)
Presiding: Cheng Lin, Eric Dodds
Room 131-132

A diverse variety of biomolecules undergo structurally and functionally significant interactions with metal ions. These interactions can be

preserved in vacuo, where the resulting metalated species can exhibit characteristics quite dissimilar from those of their protonated counterparts. In the context of gas-phase bioanalysis, these differences can provide access to unique low-energy conformations, alternative dissociation pathways, or varied electronic properties. In addition, metal ion adduction can confer distinctive isotopic features and mass defect signatures. Taken together, these considerations highlight a vast yet largely untapped potential for metal ion coordination to enhance gas-phase bioanalytical strategies based on mass spectrometry, tandem mass spectrometry, and ion mobility spectrometry. This workshop will identify areas in which metal ion adduction yields advantages for biomolecular analysis spanning a wide range of application areas addressed using mass spectrometry and allied methods. Significant focus will be placed on practical guidance as discussants and participants survey new fundamental insights and emerging biological applications involving the use of metal ion charge carriers.

03. Open Source Software Packages: Using and Making your Contributions (Bioinformatics MS Interest Group)
Presiding: Samuel Payne, Meena Choi
Room 133-134

In the last 10 years, the computational mass spectrometry research community has grown dramatically as witnessed by the number of conference sessions, posters and workshops which focus on



bioinformatics and related computational topics. As the community grows, it is essential that we work to bring cooperation and collaboration to the great minds that contribute to advancing this area of science. One critical aspect of a community of interacting scientists is open source software. Although many tools for computational mass spectrometry have recently been released as open source, there remains a limited re-use of such tools. Thus, as a community, we are not yet benefiting from open source. The purpose of this workshop is to introduce several established open source packages to the community with a special emphasis on how they can use these tools in their own development of new algorithms. We will also discuss how to create proper APIs in a tool to promote re-use.

04. Clinical Diagnostics: Translating New Mass 8. Spectrometry Approaches (Clinical Chemistry Interest Group)
Presiding: Timothy Garrett
Room 135-136

The clinical lab relies on LC-MS/MS approaches, especially triple quadrupole instrumentation, for a growing number of diagnostic approaches because of the sensitivity, selectivity and specificity that mass spectrometry (coupled with chromatography) provides. In translational research the growth of new analytical techniques such as ion mobility, mass spectrometric imaging and high-resolution mass spectrometry are widely employed. Yet the translation of these techniques to clinical diagnostics is slow because of cost, ruggedness, untested performance to name a few. However, as an example, as the cost of high-resolution instruments comes closer to the purchase of a triple quad the advantages that high resolution MS have might aid clinical diagnostics. This workshop is designed to gather scientists working on clinical translational research and clinical diagnostics to discuss the challenges associated with implementation of newer MS based technologies and offer advice into the future at the adoption of new analytical MS approaches.

05. FTMS: Successes and Challenges of Achieving Routinely High Mass Accuracy (FTMS Interest Group)
Presiding: David Kilgour, Melinda McFarland
Room 137-138

This year's workshop will be a discussion focused on the experiences of the community when trying to analyse samples, to a consistently high mass accuracy, by FTMS methods. So, which factors impact mass accuracy on FT-MS instruments and when is mass uncertainty adversely affecting your results or the confidence in your results, in practice?

A lot of the discussion about mass accuracy gets passed over because one can be quite liberal with mass accuracy when working with proteomics. But, for many applications, reliably high mass accuracy is key. In this workshop we will discuss the community's experience of the mass accuracy routinely achievable in FT-MS instruments. We will discuss our success stories, times when our mass accuracy was not what was expected and what methods are used to overcome the problems.

For example do you experience non-linearity across the mass range and wonder why why resolving power is impacted by the mass range? Do you experience changes in the accuracy of the mass measurement accuracy across a chromatographic peak or in different regions of the spectrum and how could you compensate for this? How can you compensate for changes in temperature? How do the vendors try to overcome these issues? Do you have success stories where you have been able to distinguish co-eluting or co-located molecules of similar mass because of the mass accuracy you have been able to achieve? As usual, there will be expert instrumental developers from both industry and academia to help answer your questions.

06. Exposomics Update: Success, Lessons and Future Goals (Exposomics Interest Group)
Presiding: Anthony Macherone, Skip Kingston
Room 139

The exposome compliments the genome and interrogates changes in biological response pathways resulting from exposures and integrates these with genomics and other biological information to ultimately

determine the causative factors of chronic diseases. Within the exposome paradigm, exposures are defined as all bio-active chemicals circulating in the body. Examples include dietary chemicals, drugs, pollutants, 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. The primary tools used in exposomic studies are mass spectrometry based in the liquid and the gas phases. These methodologies are supported by sophisticated commercial and open-source bioinformatics tools that tease out associations between the chemical information, the experimental variables and meta-data in what has come to be defined as exposome-wide association studies (EWAS).

Since 2010, at least 10 large scale exposome cohorts have been defined and funded in the USA, UK, EU, Japan and China and countless independent research initiatives have commenced - many focused on pre-natal, birth and early childhood exposures. This workshop will examine the results of exposomics studies reported in peer-reviewed literature over the past 2 - 3 years. The discussion will be focused on defining the strengths and weakness of the exposome paradigm, where innovation is needed and will attempt to define a path forward for exposome researchers.

08. Antibody-Drug Conjugate Research and Development: The Role of Multifaceted Mass Spectrometry (Pharmaceuticals Interest Group)
Presiding: Matt Schenauer, John Valliere-Douglass
Room 141-142

Due to the success of pharmaceutical interest group workshops since 2013, and broad interest in the use of MS in antibody drug-conjugate (ADC) research and development, we propose a similar workshop for 2017. After a short informal presentation (less than 15 minutes) the majority of the workshop will include an audience-driven discussion with the opportunity to ask questions to peers and a panel of experts. The short presentation will include a primer on ADCs, for those practicing mass spectrometry but unfamiliar with antibody therapeutics and their conjugates, and then provide a snapshot of current applications of MS analysis in the industry for ADC R&D. The organizers will have backup questions prepared for the panel and audience to start or prompt the discussion if needed. Potential areas of discussion may include initial Mab and drug assessments, bioanalytical assay development, and the scaling range of characterization required for ADCs as they progress through clinical development. Discussion may focus on Mass Spec method development, optimization, data analysis, and how this information is being applied within industry paradigms or changing them.

09. Forensics and Homeland Security Mass Spectrometry Research: A Critical Discussion between Academicians and Forensic Science Practitioners (Forensics & Homeland Security Interest Group)
Presiding: Adam B. Hall, Kenyon M. Evans-Nguyen
Room: 143-144

Mass spectrometry serves critical needs in forensics and homeland security for the detection of a wide variety of target compounds. The reliability of these approaches has significant effects on public safety, airport security and border protection. In order to remain vigilant and utilize modern MS-based technologies within these fields, more research is needed to address gaps in knowledge during casework and screening operations. Academicians conduct the majority of MS-based forensic science research. However, a virtual chasm exists in the translation of new technologies into practice. Implementation of new technologies is often hindered by the unusually rigorous demand of forensic techniques. Data generated by forensic practitioners must yield conclusions that can be stated with a very high degree of certainty to be useful in legal proceedings and must be generated at a lower cost than private industry. An awareness of the needs and limitations of the forensic science community can lead to more productive collaborations between researchers and practitioners. The topic, "The Research Lifecycle in Forensics and Homeland Security" will be a



critical discussion between academicians and practitioners and will work to establish effective communication through a panel discussion composed of casework focused practitioners as well as forensic scientists who are involved in casework, but also do some research. Both presiders are former practitioners who are current academicians active in research. The panel will consist of diverse perspectives to engage the audience and gain a better understanding of this critical need in the fields of forensics and homeland security.

10. Art and Cultural Heritage: Mass Spec Applications

Presiding: Mehdi Moini

Room 145

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.

11. Mass Spectrometry Interactive Virtual Environment (MassIVE):

Management of Big Data

Presiding: Nuno Bandeira

Room 231-234

The public availability of hundreds of terabytes of mass spectrometry data have created significant challenges for the reanalysis and reutilization of proteomics and metabolomics data. This workshop will focus on ways to make MS big data accessible and easily reusable for interpretation of newly-acquired data in labs of all sizes. In particular, we i) will discuss the relative merits and pitfalls of big data MS reanalysis using advanced approaches such as proteogenomics, spectral library and blind modification searches and ii) will explore multiple ways to integrate MS big data into labs' everyday research process, including a discussion on how to make data sharing more productive and rewarding for data generating labs.

12. Ion Trap Instrumentation for Harsh Environment and Point-of-Care Applications (Ion Trap MS Interest Group)

Presiding: Zheng Ouyang, Wei Xu

Room 235-238

Ion trap has served well as an independent mass analyzer and gas-phase reactor for ion processing in hybrid instruments. In the new round of instrument development, ion trap is losing its elite status for large instruments but becoming a superior option for miniature MS systems for on-site, in-field analysis. With the strong trend of expanding MS for biomedical applications, miniature MS instruments for point-of-care analysis shall become a new focus of the instrumentation. This workshop will start with a provocative overview of the MS instrumentation development by Prof. R. Graham Cooks, followed by a series of short technical presentations and a panel discussion.

13. Photoionization: Applications, Developments, and Discussions (Photoionization MS Interest Group)

Presiding: Ralf Zimmermann, Eleanor Riches

Room 239

Photoionization is a complementary technique to other typical mass spectrometry ionization techniques, such as electrospray (ESI), electron ionization (EI), atmospheric pressure chemical ionization (APCI), etc. There are two main photoionization approaches in use today, namely Atmospheric Pressure Photoionization (APPI) and vacuum photoionization - more commonly known as single-photon ionization (SPI). APPI is commercially available and can be routinely implemented on LC-MS systems for diverse applications, whereas SPI is currently more of a research tool, although it is finding wider acceptance in several application areas - particularly those related to environmental analyses.

In this workshop, we will discuss novel applications and developments of both types of photoionization (APPI and SPI), with an opportunity for attendees to discuss their photoionization challenges and ask questions of colleagues and expert users. There will be a series of, very brief, presentations that will serve to initiate discussion around topics of key interest, including applications of both APPI and SPI, and novel developments in these fields. The aim is to help attendees understand more about the techniques and to have the chance to troubleshoot any specific issues they have encountered, thus broadening the implementation of photoionization in laboratories worldwide.

14. A Career in Mass Spec: Options and Where to start?

(Young Mass Spectrometrists Interest Group)

Presiding: M. Violet Lee, Doug Phanstiel

Room 240-242

This workshop is intended to serve as a resource for young scientists interested in pursuing a career in the field of mass spectrometry. Come prepared for an interactive panel discussion on professional development with panelists from academia, government, and industry (domestic and foreign, biotech and pharma). Topics will be centered around fundamental training, internships, career options, and career planning and management.

15. Top-Down Proteomics

Presiding: Paul Thomas, Ying Ge

Room 243-245

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.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL





TUESDAY MORNING ORAL SESSIONS

From 6:45 am Tuesday
CORPORATE BREAKFAST SEMINARS
 Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Tuesday INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION Nuno Bandeira (UCSD) Hall D level 1

- TOA am 08:30 **PROSPEC: The PROteometools SPEctrum Compendium**; Mathias Wilhelm¹; Daniel P Zolg¹; Karten Schnatbaum²; Johannes Zerweck²; Tobias Knaute²; Bernard Delanghe³; Siegfried Gessulat¹; Hans-Christian Ehrlich⁴; Maximilian Weininger¹; Peng Yu¹; Patroklos Samaras¹; Judith Schlegel⁵; Karl Kramer¹; Tobias Schmidt¹; Holger Wenschuh²; Thomas Moehring³; Stephan Aiche⁴; Andreas F. Huhmer⁶; Ulf Reimer²; Bernhard Kuster^{1,7}.
¹Technical University of Munich, Freising, Germany; ²JPT Peptide Technologies GmbH, Berlin, Germany; ³Thermo Fisher Scientific, Bremen, Germany; ⁴SAP SE, Potsdam, Germany; ⁵SAP SE, Walldorf, Germany; ⁶Thermo Fisher Scientific, San Jose, CA; ⁷Center for Integrated Protein Science Munich, Freising, Germany; ⁸Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany
- TOA am 08:50 **False Discovery Rates are Underestimated by the Target-decoy Strategy due to Unaccounted for Chemical and Biological Modifications**; Andy Kong¹; Felipe Leprevost¹; Dmitry M. Avtonomov¹; Dattatreya Mellacheruvu¹; Alexey I. Nesvizhskii¹.
¹University of Michigan, Ann Arbor, MI
- TOA am 09:10 **PTMProphet: Highly Flexible TPP Software Enables Exploration of the Known and Unknown PTM Universe with Bayesian Mixture Modeling and Beyond**; David Shteynberg¹; Eric W. Deutsch¹; Jimmy K Eng²; Andrew Keller¹; Ulrike Kusebauch¹; Luis Mendoza¹; Zhi Sun¹; Kristian Swearingen¹; Robert L. Graham³; Julie A. Brazzatti³; Anthony Whetton³; Robert L. Moritz¹.
¹Institute for Systems Biology, Seattle, WA; ²University of Washington Genome Sciences, Seattle, WA; ³University of Manchester, Manchester, UK
- TOA am 09:30 **The Tale of Two Proteomes: How Data Processing Influences Cross-species Proteomic Analysis of Patient-derived Xenografts**; Arshag Mooradian¹; Petra Erdmann-Gilmore¹; Xuya Wang²; Qiang Zhang¹; Sandeep Rajput¹; Zhanfang Guo¹; Jeremy Hoog¹; Kelly V. Ruggles²; Sjoerd van der Post¹; Sherri R. Davies¹; David Fenyö²; Shunqiang Li¹; Gary L. Johnson³; Cynthia X. Ma¹; R. Reid Townsend¹; Jason Held¹.
¹Washington University School of Medicine, St. Louis, MO; ²New York University School of Medicine, New York, NY; ³University of North Carolina School of Medicine, Chapel Hill, NC
- TOA am 09:50 **Covariation of Peptide Abundances Accurately Reflects Protein Concentration Difference**; Bo Zhang¹; Mohammad Pirmoradian¹; Roman Zubarev¹; Lukas Käll².
¹Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Solna, Sweden; ²Royal Institute of Technology, Stockholm
- TOA am 10:10 **pLink2.0: Improved Search Engine for Large Scaled Cross-linked Peptides Identification**; Jia-Ming Meng¹; Ji-Li Yin¹; Zhen-Lin Chen¹; Sheng-Bo Fan¹; Yan-Jie Wu¹; Hao Chi¹; Chao Liu¹; Si-Min He¹.
¹ICT, CAS, Beijing, China

8:30-10:30 am Tuesday QUANTITATIVE ANALYSIS IN DRUG DISCOVERY AND DEVELOPMENT Petia Shipkova (Bristol Myers Squibb) 500 Ballroom level 1

- TOB am 08:30 **Identification Of Contamination Of Skin Tissues Using Quantitative Mass Spectrometry Imaging**; Raphael Legouffe¹; Stefan Linehan²; David Bonnel¹; Jonathan Stauber¹; ¹Imabiotech, Loos, France; ²Imabiotech Corp, Billerica, MA
- TOB am 08:50 **Pharmacokinetic and MALDI-MSI Assessment of Orally Active Analgesic Cyclopeptides and Related Therapeutics Built on the Cyclotide Scaffold**; Aaron G Poth¹; Brett R Hamilton²; Yen-Hua Huang¹; Francis C K Chiu³; Thao T Le¹; Meng-Wei Kan¹; Michelle L Colgrave⁴; Susan A Charman³; Deon J Venter²; David J Craik¹.
¹Institute for Molecular Bioscience, The University of Queensland, Brisbane, Australia; ²Mater Hospital, Brisbane, Australia; ³Centre for Drug Candidate Optimisation, Monash Institute of Pharmaceutical Sciences, Monash University, Parkeville, Australia; ⁴CSIRO, Agriculture Flagship, St Lucia, Australia
- TOB am 09:10 **Quantification of Anticancer Drug in Live Single Cancer Cells using the Single-probe Device**; Ning Pan¹; Shawna Standke¹; Zhibo Yang¹.
¹University of Oklahoma, Norman, OK
- TOB am 09:30 **Important Considerations for LC/MS-based Analysis of Tissue Distributions of Therapeutic Monoclonal Antibody**; Bo An¹; Ming Zhang¹; Jun Qu¹; Yang Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- TOB am 09:50 **Development of Quantitative Mass Spectrometry Assays for Species-matched Surrogate Antibody Fragments in Ocular Matrices**; Hilda Hernandez-Barry¹; Robert F Kelley²; Devin Tesar²; Whitney Shatz²; Laetitia Comps-Agrar²; Joyce Chan²; Keyang Xu²; Luna Liu²; Yanqiu Liu²; Mauricio Maia²; Kelly Loyet².
¹Genentech, South San Francisco, CA; ²Genentech, Inc, South San Francisco, CA
- TOB am 10:10 **Cross Platform Comparison of HRMS Instrumentation for Intact Quantitation of Biotherapeutics for PK Analysis**; Lisa A. Vasicek¹; Alex ZHU²; Daniel S. Spellman¹; Kevin Bateman¹.
¹Merck Research Labs, West Point, PA; ²Agilent Technologies, Wilmington, DE

8:30-10:30 am Tuesday QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS Wei-Jun Qian (PNNL) Sagamore 1-3 level 2

- TOC am 08:30 **Determination of Absolute Phosphorylation Stoichiometry in Human Cells by Motif-targeting Quantitative Proteomics**; Chia-Feng Tsai^{1,2}; Yen-Chen Liao^{1,3}; Yi-Ting Wang¹; Pei-Yi Lin¹; Miao-Hsia Lin¹; Alexey I. Nesvizhskii⁴; Yasushi Ishihama²; Yu-Ju Chen^{1,3}.
¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ²Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ³Department of Chemistry, National Taiwan University, Taipei, Taiwan; ⁴Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, MI
- TOC am 08:50 **Targeted Dissection of Cellular Signaling Pathways by Simultaneous TOMAHAQ on Peptides and Phosphopeptides**; Brian K. Erickson¹; Devin Schweppe¹; Joao A Paulo¹; Alison R Erickson¹; Jeffery Knott²; Steven P Gygi¹.
¹Harvard Medical School, Boston, MA; ²Cell Signaling Technologies, Danvers, MA



- TOC am 09:10 **Multiplexed Kinase Pathway Monitoring using Phosphoproteomics of Effector Transcription Factors**; Alexander Federation¹; Sandi Spencer²; James Bollinger²; John Stamatoyannopoulos¹; ²Michael J MacCoss²; ¹Altius Institute, Seattle, WA; ²University of Washington Genome Sciences, Seattle, WA
- TOC am 09:30 **A Dynamic Picture of the Ubiquitinome upon Proteasome Inactivation**; Jeroen AA Demmers¹; Karen A Sap^{1,2}; Lennart van der Wal¹; Karel Bezstarosti¹; Dick HW Dekkers¹; Olaf Voets¹; Erikjan Rijkers¹; ¹Erasmus University Medical Center, Rotterdam; ²Academic Medical Center Amsterdam, Amsterdam, Netherlands
- TOC am 09:50 **Site-specific Mapping of the Human SUMO Proteome Reveals Crosstalk with other Post-Translational Modifications**; Ivo Hendriks¹; David Lyon¹; Clifford Young¹; Lars J Jensen¹; Alfred CO Vertegaal²; Michael L Nielsen¹; ¹Novo Nordisk Foundation Center for Protein Research, København; ²Leiden University Medical Center, Leiden
- TOC am 10:10 **Proteome-wide Analysis of S-acylation Reveals Widespread Occurrence in Human Cells**; Bo Zhou¹; Yiwu Yan¹; Michael R Freeman¹; Wei Yang¹; ¹Cedars-Sinai Medical Center, Los Angeles, CA

8:30-10:30 am Tuesday
EXPOSOMICS: TARGETED, UNTARGETED AND
BIOINFORMATICS METHODOLOGIES
John Bowden (NIST)
Sagamore 4 level 2

- TOD am 08:30 **Integrated Mass Spectrometry-based Methods to Characterize Electronic Cigarette Exposure in Humans**; Romel P. Dator¹; Laura Maertens¹; Andrea Carra¹; Peter W. Villalta¹; Silvia Balbo¹; ¹University of Minnesota, Minneapolis, MN
- TOD am 08:50 **High-coverage Metabolomic Analysis of One Microliter of Blood Using Two Isotope Labelings and High-resolution LC-MS**; Wei Han¹; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada
- TOD am 09:10 **Exposure Characterization of Pesticides through Untargeted Investigation of the Urinary Exposome**; Emilien L Jamin^{1,2}; Adéline Delcambre¹; ²Jean-François Martin^{1,2}; Nathalie Bonvalot³; Emmanuelle Kesse-Guyot⁴; Jean-Pierre Cravedi¹; Laurent Debrauwer^{1,2}; ¹Toxalim (Research Centre in Food Toxicology), Toulouse University, INRA, ENVT, INP-Purpan, UPS, Toulouse, France; ²INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France; ³EHESP – School of Public Health, Rennes – Sorbonne Paris Cité, Rennes, France; ⁴Sorbonne Paris Cité Epidemiology and Statistics Research Center (CRESS), Nutritional Epidemiology Research Team (EREN), Inserm U1153, INRA U1125, Cnam, Paris13 University, Paris5 University, Paris7 University, Paris, France
- TOD am 09:30 **Gas Chromatography with Orbitrap-based High-Resolution Mass Spectrometry for Untargeted Profiling of the Human Exposome**; Douglas L. Walker^{1,2}; Yongliang Liang¹; Annette M. Esper¹; Greg S. Martin¹; Gary W. Miller²; Dean P. Jones¹; ²Division of Pulmonary, Allergy and Critical Care Medicine, Department of Medicine, Emory University, Atlanta, GA; ²HERCULES Exposome Research Center, Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA
- TOD am 09:50 **Building a Library with >1000 Ion Mobility Collision Cross Sections for Ultrafast Small Molecule Analyses**; Xueyun Zheng¹; Noor A.

- Aly¹; Vanessa L. Paurus¹; Yuxuan Zhou¹; Daniel J. Orton¹; Richard D. Smith¹; Erin S Baker¹; ¹Pacific Northwest National Laboratory, Richland, WA
- TOD am 10:10 **Exposomics Research using Suspect Screening and Non-targeted Analysis Methods and Tools at the U.S. Environmental Protection Agency**; Elin M. Ulrich¹; Jon R. Sobus¹; Antony J. Williams²; Andrew D. McEachran³; Mark J. Strynar¹; Ann M. Richard²; Christopher M. Grulke²; Seth R. Newton¹; ¹U.S. Environmental Protection Agency, National Exposure Research Laboratory, Research Triangle Park, NC; ²U.S. Environmental Protection Agency, National Center for Computational Toxicology, Research Triangle Park, NC; ³ORISE Research Participant, U.S. Environmental Protection Agency, National Center for Computational Toxicology, Research Triangle Park, NC

8:30-10:30 am Tuesday
MACROMOLECULAR COMPLEXES
Brian Chait (Rockefeller University)
Sagamore 5-7 level 2

- TOE am 08:30 **Data-driven Discovery and Validation of Human Protein Complexes via Proteome-scale Affinity-Purification Mass Spectrometry Profiling**; Edward L. Huttlin¹; Raphael J. Bruckner¹; Gabriela Zarraga¹; Joe R. Cannon¹; Lily Ting¹; Spyros Artavanis-Tsakonas²; J. Wade Harper¹; Steve Gygi¹; ¹Harvard Medical School, Boston, MA; ²Biogen, Cambridge, MA
- TOE am 08:50 **Mapping the Liver Interactome**; Mark Larence¹; Michele Tiniti²; Michael Ferguson²; Angus Lamond²; ¹The University of Sydney, Camperdown, Australia; ²University of Dundee, Dundee, UK
- TOE am 09:10 **Dynamics of the Mitochondrial Interactome**; James Bruce¹; Juan D. Chavez¹; Devin K. Schweppe¹; Xuefei Zhong¹; Chi Fung Lee¹; Arianne Caudal¹; Rudy Stuppard¹; Philip A. Kramer¹; Matthew D. Campbell¹; David J. Marcinek¹; Rong Tian¹; ¹University of Washington, Seattle, WA
- TOE am 09:30 **Endogenous Interactome of the Transcription Regulator HCF-1 Reveals Transcription Elongation as Driver of herpesvirus Reactivation from Latency**; Pierre M Jean Beltran¹; Roberto Alfonso-Dunn²; Anne-Marie W Turner²; Jesse H Arbuckle²; Hanna G Budayeva¹; Thomas M Kristie²; Ileana Cristea¹; ¹Princeton University, Princeton, NJ; ²NIH, Bethesda, MD
- TOE am 09:50 **High Resolution Mass Measurements Reveal Heterogeneity in Intact Ribosomal Particles**; Michiel van de Waterbeemd¹; Kyle L Fort¹; Dmitriy Boll²; Maria Reinhardt-Szyba²; Andrew Routh³; Alexander Makarov²; Albert J R Heck¹; ¹Utrecht University, Utrecht, Netherlands; ²Thermo Fisher Scientific, Bremen, Germany; ³University of Texas Medical Branch, Galveston, TX
- TOE am 10:10 **Charge Detection Mass Spectrometry Reveals Details of Hysteresis in Virus Capsid Disassembly**; Corinne Lutomski¹; Nicholas Lykтей²; Joseph Che-Yen Wang²; Zhongchao Zhao²; Adam Zlotnick²; Martin Jarrold²; ¹Indiana University, Bloomington, IN; ²Indiana University, Bloomington, IN

8:30-10:30 am Tuesday
ION MOBILITY: STRUCTURE
Carlos Larriba-Andaluz (IUPUI)
Wabash level 1

- TOF am 08:30 **Direct Observation of Intermediates and Structurally Distinct Products Associated with Protein Melting Transitions by Ion Mobility**



TUESDAY MORNING ORAL SESSIONS

- Spectrometry-Mass Spectrometry;** Tarick El-Baba¹; Daniel W Woodall¹; Daniel R Fuller¹; Shannon A Raab¹; Wen Liu²; Yang Liu²; Arthur Laganowsky²; David H Russell²; David E Clemmer¹; ¹Indiana University, Bloomington, IN; ²Texas A&M University, College Station, TX
- TOF am 08:50 **Effect of Time, Temperature and Humidity on Gas Phase Protein Structure;** Juan Fernandez de la Mora¹; Michel Attoui²; ¹Yale University - Mechanical Engineering Department, New Haven, CT; ²University Paris-Est Creteil, University Paris-Diderot, Paris, France
- TOF am 09:10 **Structural Dynamics of Native-like Ions: Results from Tandem Ion Mobility and Mass Spectrometry;** Samuel J. Allen¹; Rachel M. Eaton¹; Matthew F. Bush¹; ¹University of Washington, Department of Chemistry, Seattle, WA
- TOF am 09:30 **ORIGAMI: A Software Package for Data Acquisition and Analysis of Ion Mobility Collision Induced Unfolding Data from Multimeric Protein Assemblies;** Lukasz G. Migas¹; Aidan France¹; Bruno Bellina¹; Kamila J. Pacholarz¹; Perdita E. Barran¹; ¹University of Manchester, Manchester, UK
- TOF am 09:50 **The Reversible Coulombic-driven (un)Folding of Oligorotaxane Switches Probed by Ion Mobility Mass Spectrometry and Molecular Dynamics;** Emeline Hanozin¹; Benoit Mignolet²; Denis Morsa¹; Damien Sluysmans³; Anne-Sophie Duwez³; Fraser Stoddart⁴; Françoise Remacle²; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, Liège, Belgium; ²Theoretical Physical Chemistry, Liège, Belgium; ³Nanochemistry and Molecular Systems, Liège, Belgium; ⁴Mechanostereochemistry Group, Evanston, IL
- TOF am 10:10 **Conformational Sampling of GHRH 1-29 Peptide Analogs using CIA-TIMS-MS;** Kevin Jeanne Ditt Fouque¹; Luis M. Salgueiro²; Renzhi Cai²; Wei Sha²; Andrew V. Schally²; Francisco A. Fernandez-Lima¹; ¹Department of Chemistry and Biochemistry, Florida International University, Miami, FL; ²University of Miami School of Medicine/VA Medical Center, Department of Pathology and Department of Medicine, Divisions of Hematology/Oncology and Endocrinology and Sylvester Comprehensive Cancer Center, Miami, FL

8:30-10:30 am Tuesday INSTRUMENTATION: MASS ANALYZER INNOVATIONS Ryan Danell (Danell Consulting) Room 101-106 level 1

- TOG am 08:30 **Twisted Dual-field Multipole Converging Ion Guides: Achieving High Performance in Tandem Mass Spectrometers with Reduced Size;** Haopeng Wang¹; Laura L. Pollum¹; Kenneth R. Newton¹; James L. Bertsch¹; Shane E. Tichy¹; ¹Agilent Technologies, Santa Clara, CA
- TOG am 08:50 **Stimulated Motion Suppression (STMS): A New Approach to Break the Resolution barrier for Ion Trap Mass Spectrometry;** Xiaoyu Zhou¹; Xinwei Liu¹; Wenbo Cao¹; Ang Li²; Xiao Wang³; Zheng Ouyang^{1,3,4}; ¹Department of Precision Instrument, Tsinghua University, Beijing, China; ²PurSpec Technologies Inc, Beijing, China; ³Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; ⁴Department of Chemistry, Purdue University, West Lafayette, IN
- TOG am 09:10 **(Ultra-)High Resolution Multiple-Stage Tandem Mass Spectrometry (MSⁿ) in A Time-of-Flight Mass Spectrometer;** Wolfgang R Plaab^{1,2}; Wayne

- Lippert¹; Timo Dickel^{1,2}; Samuel Ayet San Andres^{1,2}; Julian Bergmann¹; Hans Geissel^{1,2}; Johannes Lang¹; Christoph Scheidenberger^{1,2}; Wolfgang Schrader³; Alessandro Vetere³; Mikhail Yavor⁴; ¹Justus Liebig University Giessen, Giessen, Germany; ²GSI Helmholtz Centre for Heavy Ion Research, Darmstadt, Germany; ³Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; ⁴Institute for Analytical Instrumentation, St. Petersburg, Russia
- TOG am 09:30 **Measuring Collisional Cross Sections of Individual Ions with Charge Detection Mass Spectrometry;** Andrew G. Elliott¹; Conner C. Harper¹; Haw-Wei Lin¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- TOG am 09:50 **Phase-coherent Ion Dispersion in Non-linear Electric Fields Enables FT-ICR MS at the Cyclotron Frequency;** Konstantin O. Nagornov¹; Edith Nicol²; Anton N. Kozhinov¹; Yuri O. Tsybin¹; ¹Spectroswiss Sàrl, Lausanne, Switzerland; ²Ecole Polytechnique, Palaiseau, France
- TOG am 10:10 **Extension of Orbitrap Capabilities to Enable New Applications;** Alexander Makarov¹; Erik Cousijn¹; Jesse Canterbury²; Eduard Denisov¹; Christian Thoeing¹; Oliver Lange¹; Arne Kreutzmann¹; Konstantin Ayzikov¹; Eugen Damoc¹; Arrey Tabiwang¹; Yue Xuan¹; Seema Sharma²; Romain Huguet²; Graeme McAlister²; Mike Senko²; Vlad Zabrouskov²; Alexander Harder¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²ThermoFisher, San Jose, CA

8:30-10:30 am Tuesday FUNDAMENTALS: ION SPECTROSCOPY Etienne Garand (University of Wisconsin) Room 107-110 level 1

- TOH am 08:30 **Water Microsolvation Switches the Binding Mode of Ni(II)Triglycine From Iminol to Charge-Solvation;** Robert C. Dunbar¹; Jonathan K. Martens²; Giel Berden¹; Jos Oomens^{2,3}; ¹Case Western Reserve Univ, Cleveland, OH; ²Radboud University, Nijmegen; ³University of Amsterdam, Amsterdam, Netherlands
- TOH am 08:50 **The Molecular Structure of Electron Transfer Dissociation Product Ions Investigated using Infrared Ion Spectroscopy;** Lisanne Kempkes¹; Jonathan Martens¹; Giel Berden¹; Jos Oomens¹; ¹FELIX Facility, Radboud University, Netherlands
- TOH am 09:10 **Analysis of Perfluorocarbons Compounds (PFCs), Potent Greenhouses Gases by Action Spectroscopy;** Suzie Douix¹; Héloïse Dossmann²; Laurent Nahon¹; Alexandre Giuliani³; ¹Synchrotron Soleil, Saint Aubin, France; ²Université Pierre et Marie Curie, Paris, France; ³Institut National de la Recherche Agronomique, Paris, France
- TOH am 09:30 **The Structure of the Anionic Serine Octamer;** Jongcheol Seo¹; Stephan Warnke¹; Kevin Pagel^{1,2}; Michael T. Bowers³; Gert von Helden¹; ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Berlin; ²Freie Universität Berlin, Berlin, Germany; ³University of California Santa Barbara, Santa Barbara, CA
- TOH am 09:50 **Conformation-Specific Infrared and Ultraviolet Spectroscopy of Cold [YAPAA+H]⁺ and [YGPAA+H]⁺ Ions: A Stereochemical "Twist" on the β -Hairpin Turn;** Andrew DeBlase¹; Christopher P. Harrila²; John T. Lawler²; Nicole L. Burke²; Scott A. McLuckey²; Timothy S. Zwier²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN

TUESDAY MORNING ORAL SESSIONS

TOH am 10:10 **Combining Mass Spectrometry, Ion Mobility and Cryogenic Ion Spectroscopy for Structural Assignment of Oligosaccharides**; Chiara Masellis¹; Neelam Khanal²; David E. Clemmer²; Michael Z. Kamrath¹; Thomas R. Rizzo¹; ¹EPFL, Lausanne, Switzerland; 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

TUESDAY AFTERNOON ORAL SESSIONS

TOA pm 02:30 **2:30-4:30 pm Tuesday**
INFORMATICS: METABOLOMICS
XiuXia Du (UNC Charlotte)
Hall D level 1
Towards a Comprehensive Virtual Research Infrastructure for Large-scale Processing of Metabolomics Data and Analysing Medical Metabolic Phenome Data; Thomas Hankemeier¹; Michael S van Vliet¹; Amy C Harms¹; Alberto Pasamontes Funez¹; Merlijn van Rijswijk²; Steffen Neumann³; Ola Spjuth⁴; Etienne Thevenot⁵; Fabien Jourdan⁶; Tim Ebbels⁷; Robert Glen⁷; Susanna-Assunta Sansone⁸; Christoph Steinbeck⁹; ¹Leiden University, Leiden, Netherlands; ²Netherlands Metabolomics Centre, Utrecht, Netherlands; ³Leibniz Institute for plant Biochemistry, Halle (Saale), Germany; ⁴Uppsala University, Uppsala, Sweden; ⁵CEA Saclay, Gif-sur-Yvette, France; ⁶INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France; ⁷Department of Surgery and Cancer, Imperial College, London, UK; ⁸Oxford e-Research Centre, Oxford, UK; ⁹EMBL-EBI, Cambridge, Cambridgeshire

TOA pm 02:50 **Hybrid Search: A Library-based Method for Identifying Metabolites Not in Tandem Mass Spectrometry Libraries**; Brian T. Cooper^{1,2}; Stephen E. Stein²; Xinjian Yan²; Yamil Simón-Manso²; Dmitrii V. Tchekhovskoi²; Yuri A. Mirokhin²; ¹UNC Charlotte, Charlotte, NC; ²NIST, Gaithersburg, MD

TOA pm 03:10 **Development of an Expert System to Enhance Gas Chromatography-Mass Spectrometry-Based Metabolite Identification**; Feng Qiu¹; Zhenhuan Lei¹; Lloyd W. Sumner¹; ¹University of Missouri, Columbia, MO

TOA pm 03:30 **Enhancing Computational Tools for Automated Ion Mobility-Mass Spectrometry-Based Small Molecule Workflows and Improved Multidimensional Analyses**; Aivett Bilbao¹; Xueyun Zheng¹; Bryson C. Gibbons¹; Ed Darland²; Emma E. Rennie²; Richard D. Smith¹; Erin S. Baker¹; Thomas O. Metz¹; John Fjeldsted²; Samuel H. Payne¹; ¹Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA; ²Agilent Technologies, Santa Clara, CA

TOA pm 03:50 **A Cellular Dashboard for Graphical Analysis of Metabolomics Data**; Peter Karp¹; Suzanne Paley¹; Paul O'Maille¹; ¹SRI International, Menlo Park, CA

TOA pm 04:10 **Untargeted Metabolomics Suffers from Incomplete Data Analysis**; Richard Baran; Baran Bioscience, LLC, Berkeley, CA

TOB pm 02:50 **High Resolution Approaches for the Identification of Environmental Metabolites**; Jeffrey Gilbert¹; Jesse L. Balcer¹; Yelena Adelfinskaya¹; David G. McCaskill¹; Shusheng Lu¹; Kyung Myung¹; Pete Johnson¹; ¹Dow AgroSciences, Indianapolis, IN

TOB pm 03:10 **A Novel Screening Workflow using Ion-Mobility-Mass Spectrometry for the Analysis of Extractable and Leachable Components from Common Packaging Material**; Jane Cooper¹; Oliver Burt¹; Baiba Cabovska²; Chris Stumpf²; ¹Waters Corp., Wilmslow, UK; ²Waters Corp, Milford, MA

TOB pm 03:30 **Identification and Relative Quantitation of Oxytocin Degradation Products under Accelerated Stress conditions using Liquid Chromatography-high Resolution Mass Spectrometry (LC-HRMS)**; Jinhui Zhang¹; Ahmed Zidan¹; Patrick J Faustino¹; ¹FDA, Silver Spring, MD

TOB pm 03:50 **An Alternate Approach to the Control of Polio Vaccine and Reference Standards using Quantitative Proteomics**; Terry D. Cyr¹; Marybeth Creskey¹; Diane Viel¹; Tong Wu¹; ¹Health Canada, Ottawa, ON, Canada

TOB pm 04:10 **A Unifying, Informatics-Based Approach to Life Cycle Management of Impurity Data in Pharmaceutical Development**; Albert Van Wyk¹; Dmitry Mityushev²; Petr Kandalov²; Graham A. McGibbon¹; Andrew A. Anderson¹; ¹ACD/Labs, Toronto, ON, Canada; ²ACD Ltd., Moscow, Russia

2:30-4:30 pm Tuesday QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY

Brad Ackerman (Eli Lilly & Co.)
Sagamore 1-3 level 2

TOC pm 02:30 **Quantitative Mass Spectrometry Analysis of PD-L1 Protein Expression, N-glycosylation and Expression Stoichiometry with PD-1 and PD-L2 in Human Melanoma**; Carlos Morales-Betanzos¹; Hyounghoo Lee¹; Paula I. Gonzalez-Ericsson¹; Justin M. Balko¹; Douglas B. Johnson¹; Lisa J. Zimmerman¹; Daniel C. Liebler^{1,2}; ¹Vanderbilt University, Nashville, TN; ²Protypia, LLC, Brentwood, TN

TOC pm 02:50 **A Method for Spatially and Temporally Resolving G Protein-coupled Receptor Protein Interaction Networks in Living Cells**; Ruth Huttenhain^{1,2}; Braden T. Lobingier¹; Kelsie Eichel¹; Alice Y. Ting³; Mark Von Zastrow¹; Nevan J. Krogan^{1,2}; ¹UCSF, San Francisco, CA; ²Gladstone Institutes, San Francisco, CA; ³Stanford University, Stanford, CA

TOC pm 03:10 **Systems Biology and Quantitative Proteomics Approaches to Studies of Mitochondrial Dysfunction for the Discovery of Friedreich's Ataxia Biomarkers**; Ian A. Blair¹; Qingqing Wang¹; Lili Guo²; Liwei Weng²; Ashkan Salamtipour¹; David R. Lynch^{3,4}; Clementina Mesaros²; ¹Penn SRP Center and Center of Excellence for Environmental Toxicology, University of Pennsylvania, Philadelphia, PA; ²Penn SRP Center and Center of Excellence

TOB pm 02:30 **2:30-4:30 pm Tuesday**
MS IN THE REGULATORY ENVIRONMENT
Whitney Stutts (FDA)
500 Ballroom level 1
Accurate Mass Fragment Library of Nootropic Compounds using DART-HRAM-MS; Sara Kern¹; Valerie M. Toomey¹; Lisa M. Lorenz¹; Jonathan J. Litzau¹; ¹USFDA Forensic Chemistry Center, Cincinnati, OH



TUESDAY AFTERNOON ORAL SESSIONS

- in *Environmental Toxicology*, University of Pennsylvania, Philadelphia, PA; ³Department of Neurology, Children's Hospital of Philadelphia, Philadelphia, PA; ⁴Department of Pediatrics, University of Pennsylvania, Philadelphia, PA
- TOC pm 03:30 **Relative Merits of Large-Scale Networks Generated by Quantitative Protein Expression Correlation and Affinity Purification – Mass Spectrometry**; David Nusinow¹; John Szpyt²; Christopher Rose²; Mahmoud Ghandi³; Edward L Huttlin²; Levi A Garraway^{3,4}; Steven P Gygi²; ¹Harvard Medical School, Boston, MA; ²Harvard Medical School, Boston, MA; ³Broad Institute of MIT and Harvard, Cambridge, MA; ⁴Dana Farber Cancer Institute, Boston, MA
- TOC pm 03:50 **Defining the Cross-talk between Signaling Pathways and Chromatin Modifications Occurring during Treatment of Acute Myeloid Leukemia**; Simone Sidoli¹; Pamela J. Sung¹; Katarzyna Kulej^{1,2}; Martin Carroll¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²The Children's Hospital of Philadelphia, Philadelphia, PA
- TOC pm 04:10 **Identification of Phosphoprotein and Phosphoprotein Networks Linked to Spine Loss in Schizophrenia**; Matthew L Macdonald¹; Megan Garver¹; Ying Ding¹; Harris Bell-Temin¹; David A Lewis¹; Robert Sweet¹; Nathan A Yates¹; ¹University of Pittsburgh, Pittsburgh, PA

2:30-4:30 pm Tuesday

ENVIRONMENTAL: NEW INSTRUMENTATION AND APPROACHES Kerri Pratt (University of Michigan) Sagamore 4 level 2

- TOD pm 02:30 **Untargeted Profiling of Soil Metal-metabolites by LC-ICPMS-ESIMS Reveals Plant-microbe Interactions**; Rene Boiteau¹; Jared B Shaw²; Ljiljana Pasa-Tolic²; ¹Pacific Northwest National Lab, Richland, WA; ²Pacific Northwest National Lab, Richland, WA
- TOD pm 02:50 **Rapid Concomitant Analysis of Pharmaceuticals in Environmental Waters by Coated Blade Spray (CBS)-Mass Spectrometry**; Justen J Poole¹; German A Gómez-Ríos¹; Ezel Boyacı¹; Nathaly Reyes Garces¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON, Canada
- TOD pm 03:10 **Detection of Volatile Disinfection By-products from Indoor Swimming Pools using a Portable GC/MS System**; Douglas Martins¹; Leonard Rorrer¹; Mitch Wells¹; Philip Tackett¹; Ernest Blatchley^{2,3}; ¹FLIR Detection, INC, West Lafayette, IN; ²Lyles School of Civil Engineering, West Lafayette, IN; ³Division of Environmental and Ecological Engineering, Purdue University, West Lafayette, IN
- TOD pm 03:30 **Liquid Overflow Capture Electrospray Ionization for the On-line Analysis of Aerosol Particles**; Kenneth D. Swanson¹; Anne L. Worth¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- TOD pm 03:50 **Real-time Molecular Analysis of Atmospheric Aerosols by Extractive Electrospray Ionization Time-of-Flight Mass Spectrometry (EESI-TOFMS)**; Felipe D Lopez-Hilfiker^{1,2}; Veronika Pospisilova²; Josef Dommen²; Joel R. Kimmel^{1,3}; Andre Prevot²; Urs Baltensperger²; Jay G. Slowik²; ¹TOFWERK, Thun, Switzerland; ²Paul Scherrer Institute (PSI), Villigen, Switzerland; ³Aerodyne Research, Inc, Billerica, MA

- TOD pm 04:10 **A New On-line Single-particle Laser Mass Spectrometer for Detection of Polyaromatic Hydrocarbons and Inorganic Constituents from the Same Individual Particles**; Ralf Zimmermann^{1,2}; Johannes Passig^{1,2}; Julian Schade¹; Matthias Fuchs²; Markus Oster²; Cornelia Jäger³; Martin Sklorz¹; ¹Joint Mass Spectrometry Centre, University of Rostock, Chair of Analytical Chemistry, Rostock, Germany; ²Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; ³Astrophysics and Cluster Physics Group, University Jena, Jena, Germany

2:30-4:30 pm Tuesday

COVALENT LABELING AND CHEMICAL CROSSLINKING Yinsheng Wang (UC Riverside) Sagamore 5-7 level 2

- TOE pm 02:30 **Protein Footprinting Probes the Protein-Membrane Interactions of Nanodisc-incorporated KRAS4b-FME**; Ben Niu¹; Don L. Rempel¹; Xiaoying Ye^{2,3}; Que Van^{2,3}; Andrew G. Stephen^{2,3}; Michael L. Gross¹; ¹Washington University, St Louis, MO; ²Frederick National Laboratory for Cancer Research, Frederick, MD; ³Leidos Biomedical Research, Inc., Frederick, MD
- TOE pm 02:50 **Mass Spectrometric Analysis of UV and Chemical protein-DNA Cross-links in a Chromatin Model**; Alexandra Stützer¹; Christin Kappert¹; Aleksandar Chernev¹; Katharina Mucek¹; Katharina Kramer²; Timo Sachsenberg³; Oliver Kohlbacher³; Wolfgang Fischle¹; Henning Urlaub¹; ¹Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; ²Max Planck Institute for Plant Breeding Research, Cologne, Germany; ³Universität Tübingen, Tübingen, Germany
- TOE pm 03:10 **The Structure of a Complete Mediator-RNA Polymerase II Preinitiation Complex Determined by Electron Microscopy and Crosslinking Mass Spectrometry**; Michael Trnka¹; Philip J Robinson²; Roger D Kornberg²; Alma L Burlingame¹; ¹UCSF, San Francisco, CA; ²Stanford University School of Medicine, Stanford, CA
- TOE pm 03:30 **Charting the Human Nuclear Protein-protein Interaction Landscape through Cross-linking Mass Spectrometry**; Domenico Fasci¹; Richard A. Scheltema¹; Albert J. R. Heck¹; ¹Utrecht University, Utrecht
- TOE pm 03:50 **Integrative Structural Proteomics of the Native Nuclear Pore Complex**; Yi Shi¹; Javier Fernandez-Martinez²; Seung Joong Kim³; Paula Upla⁴; Riccardo Pellarin³; Michael Gagnon⁵; Ilan Chemmama³; Junjie Wang²; Ilona Nudelman²; Wenzhu Zhang²; Rosemary Williams²; William Rice⁴; David L Stokes⁴; Daniel Zenklusen⁵; Andrej Sali³; Micheal P Rout²; Brian T Chait²; ¹University of Pittsburgh School of Medicine, Pittsburgh, PA; ²The Rockefeller University, New York, NY; ³University of San Francisco, San Francisco, CA; ⁴New York University School of Medicine, New York, NY; ⁵University of Montréal, Montréal, Québec
- TOE pm 04:10 **Developing an Integrated Multiplexed Quantitative Cross-linking Mass Spectrometry Platform to Determine Composition-dependent Conformational Changes of Protein Complexes**; Craig Gutierrez¹; Haibin Mao²; Clinton Yu¹; Alexander Huszaugh³; Rosa Viner⁴; Eric Novitsky³; Scott Rychnovsky³; Ning Zheng²; Lan Huang³; ¹University of California, Irvine, Irvine, CA;



²Department of Pharmacology and Howard Hughes Medical Institute, University of Washington, Seattle, WA; ³University of California, Irvine, Irvine, CA; ⁴ThermoFisher, San Jose, CA

2:30-4:30 pm Tuesday

MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION Kent Voorhees (Colorado School of Mines)

Wabash level 1

- TOF pm 02:30 **Optimization of Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry (REIMS) for the Automated and High-Throughput Analysis of Microorganisms and Clinical Samples;** Simon Cameron¹; Alvaro Perdones-Montero¹; Richard Schaffer²; Daniel Simon²; Zsolt Bodai¹; Burak Temelkuran¹; Frances Bolt¹; Kate Hardiman¹; Adam Burke¹; Emmanuelle Bardin¹; Tony Rickards^{1,3}; Alireza Abdolrasouli^{1,3}; Guang-Zong Yang¹; Monica Rebec³; Tamas Karancsi²; Zoltan Takats¹; ¹Imperial College London, London, London; ²Waters Research Center, Budapest; ³Imperial College Healthcare NHS Trust, London, UK
- TOF pm 02:50 **Translational Errors in Expression of Shiga Toxin from Pathogenic *Escherichia coli* as Measured by MALDI-TOF-TOF and Orbitrap Mass Spectrometry;** Clifton K. Fagerquist¹; William J. Zaragoza¹; ¹USDA/ARS, Albany, CA
- TOF pm 03:10 **MALDI and TLC MALDI of Intact Lipids for Characterizing Bacteria, Disease, and Product Quality;** Jackson O. Lay, Jr.¹; Rohana Liyanage¹; Jennifer Gidden¹; ¹University of Arkansas, Fayetteville, AR
- TOF pm 03:30 **Detecting Antibiotic Resistance by MALDI-TOF Analysis of Bacterial Membrane Glycolipids;** William E. Fondrie¹; Lisa M Leung²; Dudley K Strickland¹; Robert K Ernst²; David R Goodlett³; ¹University of Maryland School of Medicine, Baltimore, MD; ²University of Maryland School of Dentistry, Baltimore, MD; ³University of Maryland School of Pharmacy, Baltimore, MD
- TOF pm 03:50 **Monitoring Alterations to Bacterial Lipidome in Antimicrobial Resistance with HILIC-IM-MS;** Kelly M. Hines¹; Brian J. Werth²; Libin Xu¹; ¹Department of Medicinal Chemistry, University of Washington, Seattle, WA; ²Department of Pharmacy, University of Washington, Seattle, WA
- TOF pm 04:10 **Liquid Extraction Surface Analysis Mass Spectrometry for protein Analysis Directly from Clinical Isolates of *Staphylococcus aureus* and *Pseudomonas aeruginosa*;** Klaudia I Kocurek^{1,2}; Leanne Stones¹; Josephine Bunch²; Robin C May¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, UK; ²National Physical Laboratory, Teddington, UK

2:30-4:30 pm Tuesday

INSTRUMENTATION: INNOVATIONS IN FT-BASED MASS ANALYZERS

David Dearden (Brigham Young University) Room 101-106 level 1

- TOG pm 02:30 **The Next Dimension in Proteomics;** Peter B. O'Connor¹; Maria van Agthoven²; Yuko P. Y. Lam²; ¹University of Warwick, Coventry, West Midlands; ²University of Warwick, Coventry, UK
- TOG pm 02:50 **Frequency-tripled Detection with Minimized Contribution from other Frequency Orders and Maximized Sensitivity;** Chad R. Weisbrod¹; Lissa C. Anderson¹; Steve C. Beu¹; Greg T. Blakney¹; Nathan K. Kaiser¹; Alan G. Marshall¹

²John P. Quinn¹; Donald F. Smith¹; Christopher L. Hendrickson^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Florida State University, Tallahassee, FL

- TOG pm 03:10 **On the Utility of Higher Harmonics in Electrospray Ionization Fourier Transform Electrostatic Linear Ion Trap Mass Spectrometry;** Eric Dziekonski¹; Joshua T. Johnson¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- TOG pm 03:30 **Determination of Ion Collisional Cross Section Area in an Orbitrap Mass Analyzer;** James Sanders¹; Dustin D Holden¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TOG pm 03:50 **Coupling of the Liquid Sampling-Atmospheric Pressure Glow Discharge with an Orbitrap: A New Paradigm for High Precision Isotope Ratio Measurements;** R. Kenneth Marcus¹; Edward Hoegg²; David W. Koppenaal³; ¹Clemson University, Clemson, SC; ²Clemson University, Clemson, SC; ³Pacific Northwest National Laboratory, Richland, WA
- TOG pm 04:10 **Initial Characterization of 3D-printed High-Resolution Low Weight and Low Power Consuming Fourier transform Mass Spectrometer Based on Cassinian Ion Trap;** Eugene (Evgeny) Nikolaev^{1,2,3}; Gleb Vladimirov^{1,2,3}; Yury Kostyukovich^{1,2,3}; Oleg Kharybin^{1,2,3}; Luis Fernando Velasquez-Garcia⁴; ¹Skolkovo Institute of Science and Technology, Skolkovo, Russia; ²Institute of Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia; ³Moscow Institute of Physics and Technology, Dolgoprudnyj, Russia; ⁴Massachusetts Institute of Technology, Cambridge, MA

2:30-4:30 pm Tuesday

FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION

Glen Jackson (West Virginia University) Room 107-110 level 1

- TOH pm 02:30 **Who's in Charge? Dissociating "Charge-Replete" and "Charge-Deplete" Proteins;** Rachel O. Loo; Michael Nshanian; Hong Nguyen; Huilin Li; Joseph A Loo; ¹UCLA, Los Angeles, CA
- TOH pm 02:50 **Implementation of an Ion Carpet Array for Facile and Compact Surface-Induced Dissociation;** Joshua D. Gilbert¹; Alyssa Q. Stiving¹; Vicki H. Wysocki¹; ¹Ohio State University, Columbus, OH
- TOH pm 03:10 **Photodissociation and Radical Chemistry Shine Light on Deamidation and Protein Aging;** Dylan Riggs¹; Sonia V. Gomez¹; Ryan R Julian¹; ¹University of California, Riverside, Riverside, CA
- TOH pm 03:30 **Characterization of Antigenic Bacterial Oligosaccharides via Hybrid UVPD Activation Techniques;** Peggy E Williams¹; W. Ryan Parker¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TOH pm 03:50 **Gas-phase Ozonolysis of Ionized Cholesteryl Esters: Reaction Mechanisms, Products and Kinetics;** Sarah E Hancock¹; Alan T Maccarone¹; Stephen J Blanksby²; Todd W Mitchell¹; ¹University of Wollongong, Wollongong, NSW; ²Queensland University of Technology, Brisbane, Australia
- TOH pm 04:10 **Electron Induced Dissociation/Collision Induced Dissociation of Small Molecule Drugs;** Andrea F. Lopez-Clavijo¹; Helen J. Cooper²; ¹University of Birmingham, Birmingham, UK; ²University of Birmingham, Birmingham, UK



TUESDAY AFTERNOON ORAL SESSIONS

4:45-5:30 pm Tuesday
AWARD LECTURE
Vicki Wysocki (The Ohio State University)
Hall D level 1

Presentation of the Research Awards

- Award sponsored by Thermo Scientific by Iain Mylchreest to Peter Nemes (George Washington University).

- Award sponsored by Wasters Corporation by Lance Nicolaysen to Abraham Badu-Tawiah (The Ohio State University).



Biemann Medal

Ryan Julian
 University of California, Riverside

5:45 - 7:00 PM TUESDAY WORKSHOPS

There are light refreshments in common areas.

01. Trans-Proteomic Pipeline: New Advances and Future Developments Presiding: Luis Mendoza, Michael Hoopmann, Eric Deutsch Room 130

The workshop will begin with a brief overview of the open-source 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, integrating de novo, spectral library, and sequence database searching approaches, proteomics informatics using cloud computing infrastructure such as Amazon Web Services, analysis of post-translational modifications with PTMPProphet, and analysis of SWATH-MS data. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

02. Bioinformatic Approaches for Glycomics/ Glycoproteomics Presiding: Ron Orlando Room 131-132

Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM), and the only PTM that requires structural characterization. The diverse biological roles of glycans have created a demand for bioinformatics tools to identify individual species in the complex mixtures that often include isomeric glycans obtained from biological systems. This problem is compounded by the biosynthesis of glycoprotein glycans not being template driven like the other biopolymers (DNA, RNA, and Proteins). Bioinformatic tools are needed to better identify the roles and attributes of glycan in biological systems. In this workshop, the use of different bioinformatics tools to identify individual glycans/glycopeptides from MS data will be critically described and discussed.

03. Statistics and Bioinformatics using R Presiding: Jeffrey Jones, Ryan Benz Room 133-134

The objectives of this workshop will be to introduce the community to the R statistical programming language, specifically the integrated development environment R studio and a few select package libraries that facilitate data manipulation and plotting, along with presenting a few mass spectrometry relevant examples. We are proposing to structure the workshop around short 5-10 minute micro presentations introducing each subject followed by several minutes of open discussion. The overall goal of this workshop is to gauge the interests of ASMS attendees towards R statistical programming and to get a better understanding of how R can best serve the community.

04. Environmental Analysis: Modern Sampling Techniques and Data Analysis (Environmental Applications Interest Group) Presiding: Marc Engel, Imma Ferrer Achille Cappiello Room 135-136

When modern sampling techniques, both direct and indirect, are used to analyze complex environmental samples challenging data

sets are often generated. Our workshop will focus on the analysis of complex environmental samples and the use of data analysis tools and sampling techniques to generate the highest quality data for unequivocal identification. Three speakers will present 3-5 slides followed by discussion.

05. Hepatocytes: Current and Future Use in DMPK (DMPK Interest Group) Presiding: Philip Tiller, Mark Cancilla Room 137-138

Hepatocytes have become an integral tool in pharmaceutical research. Hepatocytes have been routinely used to generate metabolic stability/ intrinsic clearance and metabolite profile data. These assays are conducted using hepatocytes in suspension and have been, and continue to be effective assays, even though they exhibit a cell viability period of up to only 4 hours.

As more of the new chemicals being synthesized exhibit increased metabolic stability, there is a need to extend the hepatocyte incubation period to afford meaningful data. In recent years several approaches have been developed to increase the viable incubation period, such as hepatocyte relay assays, plated and co-cultured human hepatocyte systems, and these have matured, such as HepatoPak from Ascendence (Hepregen), Hurel co-cultured primary hepatocytes, 3D hepatocyte spheroids (Organovo) and the various hepatocyte relay assays (both suspension and plated). Additional in vitro assays have also been explored with these new tools such as toxicology, transporters and biliary excretion.

Discussion will revolve on how these new hepatocyte-based tools are impacting DMPK workflows, their pros and cons and real-life experience discussions from colleagues who have hands-on experience.

06. The NIH and NSF Review and Funding Process Presiding: Salvatore Sechi, Charles, Edmonds, Douglas Sheeley Room 139

Many ASMS members and conference participants are supported by the National Institutes of Health or the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH and NSF staff. Substantial time will be allotted for discussion and questions. NIH and NSF staff will also be available for individual discussions with investigators during scheduled "Office Hours" in the poster exhibit hall.

07. Proteomic Workflow: Unpublished Collective Practical Knowledge from Insiders (Analytical Lab Managers Interest Group) Presiding: Emily Chen, Allis Chien Room 140

There is no one-size-fits-all solution to the diversity of proteomic analyses that our labs handle every day. At the same time, we have to



make sensible decisions on what workflows to use, balancing scientific goals and available resources. The wisdom gained through these experiences is crucial to daily operations and consistent high-quality results, yet typically goes unpublished. This unpublished knowledge can help all of us make better decisions when performing proteomic analyses. The 2017 ASMS Analytical Lab Managers' Workshop will be dedicated to sharing these nuggets of practical wisdom. Four segments of proteomic workflows will be covered: sample preparation, liquid chromatography, mass spectrometry, and data analysis. A panel of core lab directors will introduce each topic and initiate discussion. Come join us - contribute your wisdom and learn from others in this collaborative workshop.

08. The Need for Speed: Is your LC or Mass Spectrometer the Top Gun for Improving Throughput?

(LCMS & Related Topics Interest Group)

Presiding: Erik Soderblom, Will Thompson

Room 141-142

In your current analytical workflow, is the mass spectrometer or analytical separation holding you back from higher throughput? With the increasing performance of modern MS instrumentation, including better sensitivity and scan speeds as fast as a few milliseconds, we gain the opportunity to increase either the speed in which analytes are separated prior to MS analysis or the number of analytes that are being simultaneously measured. This workshop will discuss considerations, opportunities and challenges in utilizing the increased performance of modern mass spectrometry instrumentation with various separation strategies while still maintaining quantitative fidelity within an assay. Topics will include emerging separations and MS strategies for improving throughput, with special consideration for multiplexed assay development and the challenges this presents.

09. Tracing Uncertainty in Imaging MS: Benchmarking Reproducibility, Variability, and Performance across Experiments

(Imaging MS Interest Group)

Presiding: Raf Van de Plas, Reid Groseclose

Room 143-144

Imaging MS is rapidly developing into a powerful molecular imaging modality. During its growth the focus has naturally been on developing new capabilities and increasing performance along the spatial and spectral domains. However, as the technology matures and is applied in fields such as translational medicine, pharmaceuticals, material science, and forensics, it becomes increasingly important to develop a better understanding of the technical variability in the experimental workflow. The need to exercise more advanced control over aspects such as reproducibility, stability, and variability across experiments (e.g. through systematic performance metrics) is steadily emerging across application fields, and robust solutions will be central to the long-term development of imaging MS. Various research groups have addressed the challenge of tracking and eliminating technical variation, and proposed different approaches ranging from sample preparation to instrumental and computational methods.

In this workshop, we will discuss current approaches to benchmarking and controlling reproducibility and variability across experiments. We will also try to identify the most pressing challenges ahead. The workshop will seek insight from the academic and clinical viewpoint in terms of required levels of rigor, and will also invite input from industry and governmental institutions that employ imaging MS in their assays and studies. Ultimately, we aim to discern an overall direction and set of best practices for the field, potentially complemented by a list of major challenges.

10. JASMS - Present Status and Future

Presiding: Joe Loo

Room 145

This Workshop will discuss the "nuts and bolts" of the operation of JASMS and how manuscripts are handled - from the time a manuscript is first submitted to the time the paper is published in the print journal. The important role of the manuscript reviewers in this process will be highlighted.

11. Biotherapeutics: Hot Topics

(Biotherapeutics Interest Group)

Presiding: Charles Cheng, Ashley Ruth

Room 231-234

This workshop will be a forum to discuss hot topics in the analysis of biotherapeutics by mass spectrometry. Mass spectrometry is now used for biotherapeutic analysis from discovery and throughout product development. Discussion may include a variety of topics, ranging from protein modifications, higher order structure characterization, protein batch comparability and biosimilarity, and biotherapeutic lot release testing. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed based on attendee interest and interest group survey responses.

12. HDX, Covalent Labeling & Cross Linking: State-of-the-Art and Future Directions

(HDX Covalent Labeling & Cross Linking Interest Group)

Presiding: Lan Huang, David Weis

Room 235-238

Following a short organizational meeting, the workshop will provide a forum for discussing hydrogen exchange, covalent labeling, and cross-linking approaches for protein analysis (structure, function, folding, dynamics). A panel of experts will present overviews of these three distinct approaches for MS-based characterization of higher-order protein structure. The overviews will include brief introductions to the general workflows, discussions of the strengths and weaknesses of the approaches, new developments and applications, identification of current challenges, and advice to newcomers on how to enter the fields. In addition, the panel will stimulate discussions about whether different methods can be effectively integrated for comprehensive protein analysis. There will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

13. Polymer Mass Spectrometry: Advances

(Polymeric Materials Interest Group)

Presiding: Steve Rumbelow, Christina Mastromatteo

Room 239

This workshop will be split into three sections, namely MALDI MS (current practices and approaches to method development), poster presentations and finally an open forum on questions/issues/developments in polymer analysis.

It will commence with Kevin Owens leading discussions on best practices around running MALDI MS by describing how his team run their systems at Drexel University, covering such areas as day-to-day usage, troubleshooting, method development and other potential issues that users may encounter. Delegates will be encouraged to share their experiences with this technique during this interactive session.

This is to be followed by short forum in which any delegates (particularly students) presenting posters in the Polymers Section at this conference, will be invited to give a short synopsis (no more than 3-5 minutes each) of their posters. The aim is to give these presenters an opportunity to introduce their posters and highlight any new developments or learnings. In order to keep within reasonable time constraints, potential attendees will be canvassed prior to the meeting.

Finally, delegates will be invited to ask questions about any issues with particular applications or techniques that they are either currently working on, or are interested in investigating further. This will include any discussions on shared experiences with various instrumental techniques, through to data interpretation and processing software.

14. Metabolomics: Integration into the Emerging Arena of Multi-omic Approaches

(Metabolomics Interest Group)

Presiding: John Bowden

Room 240-242

As the metabolomics field continues to mature, research continues to focus on not only improving metabolite measurement, but also more recently on how to expand application and usefulness of metabolomics data. One such approach is the adaptation of multi-omics. Multi-omics



5:45 - 7:00 PM TUESDAY WORKSHOPS

approaches aim to integrate the results of more than one 'omic' analysis, such as combining metabolomics with genomics or proteomics, in order to improve our understanding of biology. Despite its burgeoning usage, there are several considerations that the metabolomics community must interrogate, such as the potential need for new methodology and data analysis tools that must be developed for improved interpretation of multi-omic results. The experimental design must be revisited, for example, when developing methods that perform multiple omics from a single extract/extraction. Strategies to handle multi-omic data sets need to be developed, along with new ways to perform statistical analysis data and interpretation. Since metabolomics offers the phenotype, providing the most rapid measurement of health status, we need to continue exploring the nexus by which other 'omic' approaches help enhance our understanding of metabolism and more importantly, overall organism health. This workshop will provide an opportunity to discuss these the emerging concept of multi-omics as it pertains to the metabolomics community with a few short (5 min) presentations to spur discussion.

15. Mass Spectrometry and Ion Mobility: The Role of Temperature (Fundamentals Interest Group) Presiding: Michael Van Stipdonk, Victor Ryzhov Room 243-245

Temperature has a significant influence of mass spectrometry and ion mobility experiments. This is true whether considering, for example, the role of effective temperature on thermochemical measurements

using the kinetic method or the resolving power during separations by ion mobility. The purpose of the workshop is to explore the temperature by focusing on four (4) types of experiment: (a) use of linear free energy relationships and the kinetic method to measure gas-phase acidity and basicity, (b) threshold CID measurements to measure bond dissociation energies of reaction energy barriers, (c) temperature dependent measurements of reactions in quadrupole ion traps, and (d) variable temperature ion-mobility measurements. The format of the workshop will be discussion based, moderated by four experts in the respective areas: J. C. Poutsma for the kinetic method, Peter B. Armentrout for threshold CID, Scott Gronert for variable temperature ion trap experiments and Matt Bush for the role of temperature in ion mobility measurements. We hope the workshop will provide guidance for researchers designing experiments and interpreting the data that results from the application of mass spectrometry and ion-mobility in fundamental research.

**AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL**

WEDNESDAY MORNING ORAL SESSIONS

**From 6:45 am Wednesday
CORPORATE BREAKFAST SEMINARS
Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited**

8:30-10:30 am Wednesday INFORMATICS: DATA-INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS Arthur Moseley (Duke University) Hall D level 1

- WOA am 08:30 **Molecular Phenotyping of Alzheimer's Disease in Post-Mortem-Biospecimen Samples via Data Independent Acquisition;** Jason Michael Gilmore¹; Jennifer Merrihew¹; Jarrett Egerton¹; James Bollinger¹; Amarjeet Grewal²; Kathy Montine²; Thomas Montine²; Michael J MacCoss¹; ¹University of Washington Genome Sciences, Seattle, WA; ²Stanford School of Medicine, Stanford, CA
- WOA am 08:50 **LibMatic: A DIA-Umpire Based Pipeline to Generate Spectral Libraries for Targeted re-Extraction in DIA;** Guo Ci Teo¹; Dattatreya Mellacheruvu¹; Isabell Bludau²; Sumithra Urs^{3, 4, 5}; Kevin Conlon⁶; Felipe da Veiga Leprevost⁶; Ruedi Aebersold²; Venkatesha Basrur⁷; Diane Marie Simeone⁸; Alexey I. Nesvizhskii⁶; ¹Department of Pathology, University of Michigan, Ann Arbor, MI; ²ETH Zurich, Institute of Molecular Systems Biology, Zürich, Switzerland; ³Department of Surgery, University of Michigan, Ann Arbor, MI; ⁴Pancreatic Cancer Center, University of Michigan, Ann Arbor, MI; ⁵Translational Oncology Program, University of Michigan, Ann Arbor, MI; ⁶Department of Pathology, University of Michigan, Ann Arbor, MI; ⁷Department of Pathology, University of Michigan, Ann Arbor, MI; ⁸University of Michigan School of Medicine, Ann Arbor, MI
- WOA am 09:10 **Fighting Fire with Fire: Comprehensive DIA Spectral Libraries Improve Phosphopeptide Identification and Quantification by DIA;** Alvaro

- Sebastian Vaca Jacome¹; Jarrett Egerton²; Brian Searle²; Sonia Ting²; Adam Officer¹; Michael J MacCoss²; Steven A Carr¹; Jacob D Jaffe¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²University of Washington, Seattle, WA
- WOA am 09:30 **Spectral Library-free DIA (DDA-free DIA) Algorithm Applied to Data Generated on a Novel Fast Scanning Orbitrap Instrument;** Roland Bruderer¹; Lynn Verbeke¹; Oliver M. Bernhardt¹; Tejas Gandhi¹; Jan Muntel¹; Yue Xuan²; Lukas Reiter¹; ¹Biognosys, Schlieren, Zurich; ²Thermo Fisher Scientific, Bremen, Germany
- WOA am 09:50 **Scanning Quadrupole Data Independent Acquisition: A Novel Workflow for Targeted and Discovery Proteomics;** Ute Distler¹; Jörg Kuharev¹; Oliver M. Bernhardt²; Lukas Reiter²; Hannes Roest³; Gushinder Kaur-Atwal⁴; Sarah Lennon⁴; Jason wildgoose⁵; Keith Richardson⁴; Johannes PC Vissers⁴; Stefan Tenzer¹; ¹University Medical Center of the Johannes Gutenberg, Mainz, Rheinland-Pfalz; ²Biognosys, Schlieren, Zurich; ³Stanford University School of Medicine, Stanford, California; ⁴Waters Corporation, Wilmslow, UK; ⁵Waters Corp., Wilmslow, UK
- WOA am 10:10 **PCprofiler: Complex-centric Analysis of Protein Correlation Profiling Datasets;** Isabell Bludau¹; Moritz Heusel¹; Robin Hafen¹; George Rosenberger¹; Max Frank¹; Ben Collins¹; Matthias Gstaiger¹; Ruedi Aebersold¹; ¹Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland

8:30-10:30 am Wednesday FOOD SAFETY & CHEMISTRY: NON-TARGETED SCREENING Robert Sheridan (New York Dept of Agriculture & Markets Food Laboratory) 500 Ballroom level 1

- WOB am 08:30 **Decomposition/Speciation of Seafood Products by LC-HRMS with Multivariate Statistical Analysis;** Randy Self¹; Michael G. McLendon¹; ¹U.S. FDA, Bothell, WA



- WOB am 08:50 **The Advantages of Using MS/MS ALL with SWATH® Acquisition for Confident Compound Identification**; Paul C. Winkler¹; Craig Butt²; April Quinn-Paquet²; ¹Sciex, Framingham, MA; ²SCIEX, Framingham, MA
- WOB am 09:10 **Orthogonal Food Analysis by Surface Plasmon Resonance Biosensing - Mass Spectrometry**; Michel W. Nielsen¹; Sweccha Joshi²; Dick H. Hooijerink¹; Teris A van Beek²; Willem Haasnoot¹; ¹RIKILT Wageningen University & Research, Wageningen, Netherlands; ²Wageningen University, Wageningen, Netherlands
- WOB am 09:30 **Drift Tube Ion Mobility (DTIM) Assisted All Ions Data-independent Acquisition (DIA) Pesticide Screening**; Xin Ma¹; Jian zhong Li¹; ¹Agilent Technologies, Beijing, China
- WOB am 09:50 **Evaluation of GC-MS and Rapid Evaporative Ionization Mass Spectrometry (REIMS) Platforms for Classification of Lamb Meat Flavor**; Jessica Prenni¹; Adam L. Heuberger²; Corey D. Broeckling³; Linxing Yao³; Karissa Maneotis⁴; Anthony J. Midey⁵; Bindesh Shrestha⁵; James Murphy⁶; Dale Woerner⁴; ¹Colorado State University, Fort Collins, CO; ²Colorado State University Department of Horticulture and Landscape Architecture, Fort Collins, CO; ³Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; ⁴Colorado State University Department of Animal Sciences, Fort Collins, CO; ⁵Waters Corporation, Milford, MA
- WOB am 10:10 **Identification of Major Chemical Constituents in *Momordica charantia* using Liquid Chromatography-Mass Spectrometry and Its Lipase Inhibitory Activity**; Joydeb Chanda¹; Pulok Kumar Mukherjee²; Sayan Biswas²; Suvodip Banerjee²; Amit Kar²; Faraz Rashid³; Dipanakar Malakar³; Manoj Pillai³; ¹School of Natural Product Studies, Kolkata, India; ²School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, Kolkata -700 032, India, Kolkata, India; ³Sciex, Gurgaon, Haryana, India

8:30-10:30 am Wednesday
BIOMARKERS: QUALITATIVE ANALYSIS
Sharon Pittner (Stanford University)
Sagamore 1-3 level 2

- WOC am 08:30 **Chemically Supervised, Non-Chromatographic Accelerated Small Molecule Biomarker Discovery by Multiple Reaction Monitoring (MRM) – Profiling**; Christina Ferreira¹; Karen E Yannell¹; Tiago JP Sobreira¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- WOC am 08:50 **A Statistical Analysis into the Role of Chemical Signaling in Giant Panda Mating**; Abbey Wilson¹; Ashli Brown Johnson¹; Darrell Sparks¹; Stephan Baumann²; ¹Mississippi State University, Starkville, MS; ²Agilent Technologies, Inc., Alpharetta, GA
- WOC am 09:10 **The Proteomic and Metabolomic Characterization of Exercise-Induced Sweat**; Sean Harshman¹; Rhonda Pitsch²; Brian Geier³; Molly Fischer⁴; Maegan O'Connor⁴; Jason Eckerle⁵; Adam Strang³; Jennifer Martin³; ¹UES Inc, Air Force Research Laboratory, WPAFB, OH; ²Henry M. Jackson Foundation, Frederick, MD; ³Air Force Research Laboratory, WPAFB, OH; ⁴Oak Ridge Institute of Science & Education, WPAFB, OH; ⁵InfoSciTex Corporation, WPAFB, OH
- WOC am 09:30 **Is Proteomics Classification of Fertilized Cells Possible - A Case Study**; Goran Mitulovic¹; Tanja Panić-Janković¹; Jadranka Miletić²; Thomas Ebner³; ¹Medical University of Vienna, KIMCL, Vienna, Austria;

- ²Institute of Nuclear Sciences Vinča, Vinča, Serbia;
³Kepler Universitätsklinikum GmbH, Linz, Austria
- WOC am 09:50 **Fluorescence-Activated Cell Sorting (FACS) Coupled to Top-down Mass Spectrometry allows Cell- and Proteoform-resolved Quantitation of Lymphocytic Lineage Biomarkers**; Kristina Srzentic¹; Timothy K. Tobey¹; Paul Thomas¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL
- WOC am 10:10 **Unraveling the Complexity of The Gut-Brain Axis N-glycoproteome**; Mariana Barboza¹; Gege Xu²; Melanie Gareau¹; Helen Raybould¹; Carlito Lebrilla²; ¹Department of Anatomy, Physiology & Cell Biology, School of Veterinary Medicine, Davis, CA; ²Department of Chemistry, University of California, Davis, Davis, CA

8:30-10:30 am Wednesday
LIPIDOMICS: LIPIDS AND PROFILING
Gavin Reid (University of Melbourne)
Sagamore 4 level 2

- WOD am 08:30 **Bioactive Lipids as Clinical Biomarkers of the Inflammatory and Resolution Phases During Severe Influenza Infection**; Veronica Anania¹; Qingling Li¹; Jenny Jiang¹; Carrie M. Rosenberger¹; Wendy Sandoval¹; Adrienne Randolph²; Jacqueline M. McBride¹; W. Rodney Mathews¹; ¹Genentech, Inc, South San Francisco, CA; ²Children's Hospital Boston and Harvard Medical School, Boston, MA
- WOD am 08:50 **Lipidome Isotope Labeling of Yeast (LILY) – The Potential of ¹³C Reference Lipids for Quantitative Lipidomics Workflows**; Evelyn Rampler¹; Cristina Coman²; Gerrit Hermann^{3,4}; Robert Ahrends²; David Peake⁵; Bernard Delanghe⁶; Gunda Koellensperger⁷; ¹University Vienna, Vienna, Austria; ²Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; ³ISOTOPIC Solutions, Vienna, Austria; ⁴University of Vienna, Vienna, Austria; ⁵Thermo Fisher Scientific, St. Jose, Austria; ⁶Thermo Fisher Scientific, Bremen, Germany; ⁷University of Vienna, Vienna, Austria
- WOD am 09:10 **Harmonization of Lipidomics: Final Report of the NIST Interlaboratory Exercise on Lipidomics using Standard Reference Material 1950**; John A. Bowden¹; Alan Heckert²; Candice Z. Ulmer¹; Christina Jones¹; Jeremy Koelmel³; ¹NIST, Charleston, SC; ²NIST, Gaithersburg, MD; ³University of Florida, Gainesville, FL
- WOD am 09:30 **Endometrial Cancer Tissue Identification by Desorption Electrospray Ionisation (DESI) Imaging**; Olivia Raglan^{1,2}; Luisa Doria¹; Renata F Soares¹; James McKenzie¹; Zoltan Takats¹; Maria Kyrgiou^{1,2}; ¹Imperial College London, London; ²Imperial College Healthcare NHS Trust, London, UK
- WOD am 09:50 **Comprehensive and Quantitative Lipidomic Analysis of Human Sebum**; Elizaveta Freinkman¹; Richard J. Robinson¹; Kelli D. Goodman¹; Anne M. Evans¹; Luke A.D. Miller¹; ¹Metabolon, Inc., Durham, NC
- WOD am 10:10 **Dynamic Cell Surface Glycolipidome Revealed by nanoLC chip-Q-TOF Mass Spectrometry**; Maurice Wong¹; Gege Xu¹; Dayoung Park¹; Mariana Barboza¹; Carlito Lebrilla¹; ¹University of California, Davis, Davis, CA

8:30-10:30 am Wednesday
GLYCOPEPTIDES AND GLYCOPROTEINS
Joe Zaia (Boston University School of Medicine)
Sagamore 5-7 level 2

- WOC am 08:30 **Deglycosylation by the Acidic Glycosidase PNGase H+ Enables Analysis of N-linked Glycoproteins by Hydrogen/Deuterium Exchange Mass Spectrometry**; Jeppe B. Madsen¹; Josef



WEDNESDAY MORNING ORAL SESSIONS

- WOE am 08:50 Voglmeir²; Gerard Comamala³; Ya-Min Du²; Pernille F. Jensen⁴; Eva C. Østerlund¹; Morten B. Trelle¹; Kasper D. Rand⁴; Thomas J.D. Jørgensen¹; ¹Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; ²Glycomics and Glycan Bioengineering Research Center, College of Food Science and Technology, Nanjing Agricultural University, Nanjing, China; ³Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ⁴Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark
- WOE am 09:10 **Comprehensive Analysis of HIV Glycosylation by Capillary Electrophoresis Separation and Ultraviolet Photodissociation**; Jolene K Diedrich^{1,2}; John R. Yates III^{1,2}; ¹The Scripps Research Institute, La Jolla, CA; ²Salk Institute for Biological Studies, La Jolla, CA
- WOE am 09:30 **Thousands of Glycosites Characterized via Intact Glycopeptide Analysis using Activated Ion Electron Transfer Dissociation**; Nicholas M. Riley¹; Alexander S. Hebert¹; Michael S. Westphall¹; Joshua J. Coon¹; ¹University of Wisconsin-Madison, Madison, WI
- WOE am 09:30 **Development of Combined Phosphoproteomic and Glycoproteomic Workflows using EThcD Fragmentation**; Matthew S. Glover¹; Qing Yu¹; Zhengwei Chen¹; Lingjun Li¹; ¹University of Wisconsin Madison, Madison, WI
- WOE am 09:50 **A Novel Hybrid Platform Coupling Reverse Phase Glycoprotein Array with LC-MS/MS to Profile Glycoproteins for Cancer Biomarker Discovery and Validation**; Li Pan¹; Hillary Andaluz Aguilar¹; Linna Wang¹; Anton Iliuk^{1,2}; Andy Tao^{1,2}; ¹Purdue University, West Lafayette, IN; ²Tymora Analytical Operations, West Lafayette, IN
- WOE am 10:10 **Single Amino Acid Resolution of Glycosites with Top-down UVPD of Glycoproteins**; Catherine Going¹; Romain Huguet²; Daniel Lopez Ferrer²; Vlad Zabrouskov²; Andreas F. Huhmer²; Sharon Pitteri¹; ¹Stanford University School of Medicine, Palo Alto, CA; ²ThermoFisher, San Jose, CA

8:30-10:30 am Wednesday

IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT

Ben Bowen (Lawrence Berkeley National Lab)

Wabash level 1

- WOF am 08:30 **Chemical and Topographical 3D-surface Imaging of non-planar Objects on the Micrometer Scale Using AP-SMALDI MSI**; Bernhard Spengler¹; Mario Kompauer¹; Sven Heiles¹; ¹Analytical Chemistry, Giessen
- WOF am 08:50 **Quantitative Secondary Ion Mass Spectrometry Imaging of Chemically Communicating Microbial Communities**; Sage J. B. Dunham¹; Joseph F. Ellis¹; Nameera F. Baig^{2,3}; Nydia Morales-Soto⁴; Joshua D. Shrout^{4,5}; Paul W. Bohn^{2,3}; Jonathan V. Sweedler¹; ¹Department of Chemistry and the Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL; ²Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; ³Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN; ⁴Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN; ⁵Department of Biological Sciences, University of Notre Dame, Notre Dame, IN
- WOF am 09:10 **Emerging Modalities for Quantitative Mass Spectrometry Imaging at Atmospheric Pressure**

- WOF am 09:30 **and in Vacuum**; Akos Vertes¹; Sylwia A. Stopka²; Xavier A. Holmes²; Pranav Balan²; ¹George Washington University, Washington, DC; ²The George Washington University, Washington, DC
- WOF am 09:50 **Analysis of Tryptic Peptides and Polar Metabolites from FFPE Tissue by MALDI and LAESI MSI**; Erin H Seeley¹; Candice M Brown²; Callee M Walsh¹; ¹Protea Biosciences, Morgantown, WV; ²West Virginia University School of Medicine, Morgantown, WV
- WOF am 10:10 **Imaging and in-vivo Tissue Analysis by Infrared Laser Assisted Rapid Evaporative Ionisation MS-towards an Integrated MS-based Tissue Identification System**; Haixing Wang¹; Zsolt Bodai¹; Eftychios Manoli¹; Julia Abda¹; Dipa Gurung¹; Burak Temelkuran¹; Ed St. John¹; Daniel Leff¹; Guang-Zhong Yang¹; Zoltan Takats¹; ¹Imperial College London, London
- WOF am 10:10 **Microscope Ion Imaging of Complex Surfaces Using the Pixel Imaging Mass Spectrometry Camera**; Robert Burleigh¹; Ang Guo¹; Felix Allum¹; Michael Burt¹; Mark Brouard¹; Steve Thompson²; ¹Physical & Theoretical Chemistry Department, University of Oxford, Oxford, UK; ²Scientific Analysis Instruments Limited, Manchester, UK

8:30-10:30 am Wednesday

INSTRUMENTATION: MS IN EXTREME ENVIRONMENTS

Tim Short (SRI International)

Room 101-106 level 1

- WOG am 08:30 **Field Deployable MS for Comprehensive Atmospheric Chemistry Studies**; Benoit Plet¹; Fred Stroth²; Manjula R. Canagaratna³; Joel Thornton⁴; Jordan E. Krechmer^{3,5,6}; John T. Jayne³; Douglas R. Worsnop^{3,7}; ¹TOFWERK, Thun, Switzerland; ²Institute of Energy and Climate Research – Stratosphere (IEK-7), Research Centre Jülich GmbH, Jülich, Germany; ³Center for Aerosol and Cloud Chemistry, Aerodyne Research, Billerica, MA; ⁴University of Washington, Seattle, WA; ⁵Cooperative Institute for Research in Environmental Sciences (CIRES), Boulder, CO; ⁶Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO; ⁷Department of Physics, University of Helsinki, Helsinki, Finland
- WOG am 08:50 **Development of Portable GC/MS System with Benchtop Performance for Critical DoD Applications**; Leonard Rorrer¹; Philip Tackett¹; Daniel Sutton¹; Krystal Roark¹; Brent Rardin¹; Mitch Wells¹; ¹FLIR Detection, INC, West Lafayette, IN
- WOG am 09:10 **Development of AC Frequency Scanning in Quadrupole Ion Traps for Planetary Exploration**; Dalton T Snyder¹; Christopher J Pulliam¹; Joshua Wiley²; Jason Duncan³; Graham Cooks¹; ¹Purdue University, West Lafayette, IN; ²California Institute of Technology, Pasadena, CA; ³Acuity Brands Lighting, Inc., Crawfordsville, IN
- WOG am 09:30 **Multipole Field Effects on Cylindrical Ion Trap Performance at High Background Pressures**; Dmitriy Chernookiy¹; J. Michael Ramsey¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- WOG am 09:50 **Experimental Design for Studying High Velocity Molecular Impacts in the Gas Phase**; Anupriya Anupriya¹; Sandra Osburn¹; Brandon Turner¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT
- WOG am 10:10 **Environmental Testing and Performance Verification of the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer Under Simulated Martian Conditions**; Ryan M.

WEDNESDAY MORNING ORAL SESSIONS



Danell¹; Veronica T. Pinnick²; Andrej Grubisic³; Friso H.W. van Amerom⁴; Xiang Li⁵; Desmond A. Kaplan⁶; Ricardo D. Arevalo²; Stephanie A. Getty²; William B. Brinkerhoff²; ¹Danell Consulting, Inc., Winterville, NC; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, College Park, MD; ⁴Mini-Mass Consulting, Inc, Hyattsville, MD; ⁵Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, Baltimore County, MD; ⁶KapScience LLC, Tewksbury, MA

8:30-10:30 am Wednesday FUNDAMENTALS: PHOTOIONIZATION AND PHOTODISSOCIATION Frank Turecek (University of Washington) Room 107-110 level 1

- WOH am 08:30 **Ultraviolet Activation of Peptides Using a Tunable Photon Source**; Alexandre Giuliani¹; ²Francis Canon³; Aleksandar R. Milosavljevic¹; Laurent Nahon¹; ¹Synchrotron Soleil, Gif-sur-yvette, Essonne; ²INRA, UAR1008, Nantes, France; ³INRA, CSGA, Dijon, France
- WOH am 08:50 **Optimization of Fixed-charge and Photo-labile Derivatives for Lipid Structure Elucidation by Photodissociation**; Venkateswara R. Narreddula¹; Nathan R. B. Boase¹; Berwyck L. J. Poad¹; David L. Marshall¹; Todd W. Mitchell²; Adam J. Trevitt²; Stephen J. Blanksby¹; ¹Queensland University of

- Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia
- WOH am 09:10 **Exploration of Peptide Fragmentation Utilizing 213 nm Photons for UVPD and RDD**; Lance E. Talbert¹; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA
- WOH am 09:30 **Disentangling Radical Rearrangement Chemistry via Labile Sites and Infrared Ion Spectroscopy**; Ning Zhao¹; Karnamohit Ranka¹; John Stanton¹; Nicolas Polfer¹; ¹University of Florida, Department of Chemistry, Gainesville, FL
- WOH am 09:50 **Improved de novo Sequencing of Protonated and Charge Tagged Peptides using 157 nm VUV Photodissociation**; Nick DeGraan-Weber¹; James P. Reilly¹; ¹Indiana University, Bloomington, IN
- WOH am 10:10 **Smashing It All Up (carefully!) - Combining Surface-Induced Dissociation, Ion Mobility and UV Photodissociation as a Protein Structure Interrogation Toolbox**; Alina Theisen¹; Bruno Bellina¹; Bin Yan¹; Ines Camacho¹; Alex Jones¹; Perdita Barran¹; ¹University of Manchester, Manchester, UK

**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 INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS Kelly Ruggles (NYU School of Medicine) Hall D level 1

- WOA pm 02:30 **Metaproteomics For The Future: Democratizing Functional Analysis of Microbiomes via Community-based Informatics Development and Dissemination**; Pratik Jagtap¹; Bjoern Gruening²; James Johnson³; Alessandro Tanca⁴; Bart Mesuere⁵; W Judson Hervey⁶; Carolin Kolmeder⁷; Thomas Doak^{8,9}; Thilo Muth¹⁰; Dave Clements¹¹; Praveen Kumar¹; Thomas McGowan¹; Clemens Blank²; Bernhard Renard¹⁰; Josh Elias¹²; Joel Rudney¹; Timothy Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²Bioinformatics Group, Department of Computer Science, University of Freiburg, Freiburg, Germany; ³University of Minnesota, Minneapolis, MN; ⁴Porto Conte Ricerche, Science and Technology Park of Sardinia, Alghero, Italy; ⁵Ghent University, Ghent, Belgium; ⁶Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC; ⁷University of Helsinki, Helsinki, Finland; ⁸Indiana University, Bloomington, IN; ⁹National Center for Genome Analysis (NCGAS), Bloomington, IN; ¹⁰Robert Koch Institute, Berlin, Germany; ¹¹Johns Hopkins University, Baltimore, MD; ¹²Department of Chemical & Systems Biology, Stanford University, Stanford, CA
- WOA pm 02:50 **Personalized Profiling of Diabetes: Longitudinal Multi-omics Profiles Provide Insight into Insulin Resistance**; Hannes Roest¹; Brian Piening¹; Wenyu Zhou¹; Kevin Contrepolis¹; Gucci Gu¹; Tejaswini Mishra¹; Blake Hanson²; Eddy Bautista²; Shana Leopold²; Christine Yeh¹; Daniel Spakowicz²; Kimberly Kukurba¹; Dalia Perelman¹; Colleen Craig¹; Denis Salins¹; Sharon Pitteri¹; Tracey McLaughlin¹; George Weinstock²; Mike Snyder¹; ¹Stanford University School of Medicine, Palo Alto, CA; ²The Jackson Laboratory for Genomic Medicine, Farmington, CT
- WOA pm 03:10 **Gene Expression and Metabolomics Integration Method Defines Cancer-Specific Molecular Signatures**; Jalal K Siddiqui¹; Elizabeth Baskin¹; Russell Bonneville¹; Ewy Mathe¹; ¹Ohio State University, Columbus, OH
- WOA pm 03:30 **Unknown Protein Isoforms Resulting from Alternative pre-mRNA splicing Identified by the Integration of Mass Spectrometry and RASL-seq**; Laura Agosto^{1,2,3}; Simone Sidoli^{1,3}; Michael J. Mallory¹; Kristen W. Lynch^{1,2}; Benjamin A. Garcia^{1,2,3}; ¹Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, PA; ²Graduate Group in Biochemistry and Molecular Biophysics, University of Pennsylvania, Philadelphia, PA; ³Penn Epigenetics Institute, Dept. of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- WOA pm 03:50 **Antibody Repertoire Construction for Colorectal Cancer to Identify Tumor Affinity Antibody Peptides**; Seong Won Cha¹; Vineet Bafna¹; ¹UCSD, La Jolla, CA
- WOA pm 04:10 **A New Network Module in the Perseus Software for the Analysis of Diverse Omics Data**; Jan Rudolph¹; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany



WEDNESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Wednesday FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS

Christine Parker (FDA - Food Safety and Nutrition)
500 Ballroom level 1

- WOB pm 02:30 **Multi-Allergen Detection in Thermally Processed Baked Goods with Liquid Chromatography-Tandem Mass Spectrometry: A Comparison of Methods for Allergen Quantification;** Chelsea M. Coffey¹; Timothy R. Croley¹; ¹U.S. Food and Drug Administration, College Park, MD
- WOB pm 02:50 **Developing a Targeted Parallel Reaction Monitoring Method for the Detection of Milk-Derived Ingredients in Complex Matrices;** Michael Krawitzky¹; Charles Yang²; Melanie Downs¹; ¹University of Nebraska-Lincoln, Lincoln, NE; ²Thermo Fisher Scientific, San Jose, CA
- WOB pm 03:10 **Fingerprinting NIST Human Milk reference Material (SRM 1953) by HILIC-MS/MS for the Development of Prebiotic Oligosaccharides Mass Spectral Library;** Connie Remorosa¹; M. Lorna A De Leoz¹; Stephen E Stein¹; ¹NIST, Gaithersburg, MD
- WOB pm 03:30 **Quantification of Fructose-Asparagine, an Acrylamide Precursor, in Human Foods, Animal Foods and Mouse Ceca;** Jikang Wu¹; Anice Sabag-Daigle¹; Brian Ahmer¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- WOB pm 03:50 **Selective Detection and Quantification of Cyanotoxins in Algae Dietary Supplements using Alternative HRMS Strategies;** Audrey Roy-Lachapelle^{1,2}; Morgan Sollic³; Maryse Bouchard¹; Sébastien Sauvé¹; ¹Université de Montréal, Montréal, QC, Canada; ²Environment and Climate Change Canada, Montreal, QC, Canada; ³École Polytechnique de Montréal, Montréal, QC, Canada
- WOB pm 04:10 **Automated High Throughput Analysis of Food Products Using REIMS and Tecan EVO System – Goose or Duck Liver Paté?;** Julia Balog^{1,2}; Richard Schaffer¹; Steven Pringle^{2,3}; Zoltan Takats²; ¹Waters Research Center, Budapest; ²Imperial College London, London, London; ³Waters Corporation, Wilmslow, UK

2:30-4:30 pm Wednesday ANTIBODIES AND ANTIBODY DRUG CONJUGATES Yinyin Li (Rockefeller University) Sagamore 1-3 level 2

- WOC pm 02:30 **Screening Synthetic Fabs against Ebola and Marburg Virus Antigens by Native Mass Spectrometry and Hydrogen-Deuterium Exchange Mass Spectrometry;** Liuqing Shi¹; Parmeshwar Amatya²; Daisy W. Leung²; Gaya K. Amarasinghe²; Michael L. Gross³; ¹Washington University in St Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³Washington University in St. Louis, St. Louis, MO
- WOC pm 02:50 **Ion Mobility-Mass Spectrometry and Gas-phase Unfolding for the Quantitative Characterization of Antibody Drug Conjugates;** Yuwei Tian¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- WOC pm 03:10 **Proteomic Analysis of Serum Antibody Repertoire Dynamics Post-immunization;** Stefano Bonissone¹; Katherine Harris²; Nathan Trinklein²; Natalie Castellana¹; ¹Digital Proteomics, LLC., La Jolla, CA; ²TeneoBio, Menlo Park, CA
- WOC pm 03:30 **Complete de novo Sequencing of Monoclonal Antibodies by Mass Spectrometry;** Yongsheng Xiao¹; Monika Vecchi¹; Benbo Gao¹; Ru Wei¹; Dingyi Wen¹; ¹Biogen, Cambridge, MA

- WOC pm 03:50 **Evaluation of Peptide Mapping for Identification and Quantitation of clips in Therapeutic Proteins;** Pavel V. Bondarenko¹; Andrew Nichols¹; Da Ren¹; Lan Li¹; Jiu-Li Song¹; Le Zhang¹; Izydor Apostol¹; Zhongqi Zhang¹; ¹Amgen, Inc., Thousand Oaks, CA

- WOC pm 04:10 **Worldwide Interlaboratory Study on Monoclonal Antibody Glycosylation: Variability and Best Values;** M. Lorna A De Leoz¹; David L Dwever¹; Stephen E Stein¹; ¹National Institute of Standards & Technology, NIST, Gaithersburg, MD

2:30-4:30 pm Wednesday LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS Qibin Zhang (UNC Greensboro) Sagamore 4 level 2

- WOD pm 02:30 **Letting Ozone-induced Dissociation Out of the Box: A Modular, Platform-Independent System for Implementation in Diverse Lipidomics Workflows;** Berwyck L. J. Poat¹; Stephen J. Blanksby¹; David L. Marshall¹; Reuben S. Young¹; Todd W. Mitchell²; J. Larry Campbell³; Eva Duchoslav³; Martin R. Green⁴; Jayne Kirk⁴; Nick Tomczyk⁴; Shane R. Ellis⁵; Martin R. L. Paine⁵; Ron M. A. Heeren⁵; ¹Queensland University of Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia; ³SCIEX, Concord, ON, Canada; ⁴Waters Corporation, Wilmslow, UK; ⁵Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands
- WOD pm 02:50 **A Complete Lipidomic Approach with Capability of Quantifying C=C Location Lipid Isomers;** Wenpeng Zhang¹; Yu Xia²; Zheng Ouyang^{1,2,3}; ¹Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; ²Department of Chemistry, Purdue University, West Lafayette, IN; ³State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China
- WOD pm 03:10 **Precise Structural Characterization of Unsaturated Lipids by 213 nm UV-Photodissociation MSn;** Gavin E Reid¹; Reiko Kiyonami²; Romain Huguet²; Christopher Mullen²; Seema Sharma²; Jesse Canterbury²; Jae Schwartz²; Vlad Zabrouskov²; David Peake²; ¹School of Chemistry - University of Melbourne, Parkville, Australia; ²Thermo Fisher Scientific, San Jose, CA
- WOD pm 03:30 **Ultra-sensitive, Ultra-high Resolution Lipid and Glycolipid Isomer Analyses with a Multi-pass SLIM TWIM-MS platform and CRIMP Technology;** Roza Wojcik¹; Ian K. Webb¹; Liulin Deng¹; Jennifer E. Kyle¹; Kent J. Bloodworth¹; Noor A. Aly¹; Sandilya Garimella¹; Spencer S. Prost¹; Randolph V Norheim¹; Karl K. Weitz¹; Yehia M Ibrahim¹; Erin S Baker¹; RICHARD D. Smith¹; ¹PNNL, Richland, WA
- WOD pm 03:50 **Pulling Images from the Noise: Improving Sensitivity for Low-abundant Lipids through Gas Phase Fractionation and Enrichment;** Jeffrey M Spraggins^{1,2,3}; Raf Van de Plas^{1,2,4}; Etienne Waelkens^{5,6}; Richard M. Caprioli^{1,2,3,7,8}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Biochemistry, Vanderbilt University, Nashville, TN; ³Department of Chemistry, Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Dept. of Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; ⁶Sybioma,



KU Leuven, Leuven, Belgium; ⁷Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁸Department of Medicine, Vanderbilt University, Nashville, TN

- WOD pm 04:10 **Comparison of Quadrupole and Ion Trap Collision Induced Dissociation for Structure Determination of *Francisella Nnovicida* Lipid A variants.**; Alison Scott¹; Sung Hwan Yoon¹; Benjamin L. Oyler²; Jared B Shaw³; Dusan Velickovic³; Ljiljana Pasa-Tolic³; Robert K. Ernst¹; David Robinson Goodlett⁴; ¹University of Maryland School of Dentistry, Baltimore, MD; ²University of Maryland School of Medicine, Baltimore, MD; ³Pacific Northwest National Laboratory, Richland, WA; ⁴University of Maryland School of Pharmacy, Baltimore, MD

2:30-4:30 pm Wednesday
BIOMARKERS: QUANTITATIVE ANALYSIS
John Koomen (Moffitt Cancer Center)
Sagamore 5-7 level 2

- WOE pm 02:30 **Development and Validation of Total and Isoform-specific Assays for Quantification of Periostin in Human Serum Using Immunocapture-LC-MS/MS;** Dean E McNulty¹; Dana Knecht¹; Jonathan Kehler¹; Christopher A Evans¹; Matthew Szapacs¹; ¹GSK, King of Prussia, PA
- WOE pm 02:50 **Systematic Evaluation of SRM-, PRM- and DIA-Based Targeted Quantification;** Ehwang Song¹; Tujin Shi²; Hui Wang²; Anil K. Shukla²; Thomas L. Fillmore²; Yuqian Gao²; Ronald J. Moore²; Matthew J. Gaffrey²; Athena A. schepmoes²; Karin D. Rodland²; Richard D. Smith²; Wei-Jun Qian²; Tao Liu²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA
- WOE pm 03:10 **Detection of Ovarian Cancer Recurrence Using a Novel Integrated Proteomics Approach;** Ankit Sinha¹; Ali Hussain¹; Kwan Tang²; Vladimir Ignatchenko²; Alexandr Ignatchenko²; Blaise Clarke²; Marcus Bernardini²; Benjamin Neel³; Laurie Ailles²; Thomas Kislinger²; ¹University of Toronto, Toronto, ON, Canada; ²Princess Margaret Cancer Centre, Toronto, ON, Canada; ³Perlmutter Cancer Center, NYU Langone Medical Center, New York, NY
- WOE pm 03:30 **Development of Protein Biomarkers for Radiation Injury Using Quantitative Proteomics and Mass Spectrometry;** Kate Liu¹; Elizabeth Singer¹; Whitaker Cohn¹; William McBride¹; Julian Whitelegge¹; Joseph A Loo¹; ¹UCLA, Los Angeles, CA
- WOE pm 03:50 **Robust and Multiplexed Immuno-MRM Workflow for Relative Quantitation of Tumor Suppressors and Phosphopeptide Biomarkers of DNA Damage Response (DDR) Pathway;** Si Mou¹; Lei Xiong¹; Jeffery R. Whiteaker²; Lei Zhao²; Yihan Li¹; Amanda G. Paulovich²; Hua-Fen Liu¹; Christie Hunter¹; ¹SCIEX, Redwood City, CA; ²Fred Hutchinson Cancer Research Center, Seattle, WA
- WOE pm 04:10 **Translational Top-down Proteomics as a Path Forward to Improved Diagnostics in Human Solid Organ Transplant Rejection;** Tim Toby¹; Paul Thomas²; Josh Levitsky³; John Friedewald³; Michael Abecassis³; Neil L Kelleher²; ¹Northwestern University-Kelleher Research Group, Evanston, IL; ²Northwestern University, Chicago, IL; ³Northwestern University Feinberg School of Medicine, Chicago, IL

2:30-4:30 pm Wednesday
IMAGING: COMPUTATIONAL METHODS AND ANALYSIS
Erin Seeley (Protea Biosciences)
Wabash level 1

- WOF pm 02:30 **MSIpad: An Effective Tool for Mass Spectrometry Metabolic Imaging, as Demonstrated by Extraction of Hormone Abnormalities in Diabetic Mouse Pancreas;** Xian Mao¹; Tine Hectors²; Gerard Griffioen²; Bart De Moor¹; Etienne Waelkens³; ¹KU Leuven, ESAT-STADIUS / imec, Leuven, Belgium; ²reMYND, Bio-Incubator, Leuven, Belgium; ³KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium
- WOF pm 02:50 **Software Development for Automated Statistical Classification of Clinical Samples using Ambient Mass Spectrometry;** Jonathan H Young¹; John Lin¹; Rob Tibshirani²; Livia S Eberlin¹; ¹Department of Chemistry, The University of Texas at Austin, Austin, TX; ²Departments of Biomedical Data Sciences and Statistics, Stanford, CA
- WOF pm 03:10 **Data Dependent Imaging Mass Spectrometry of Serial Tissue Sections Guided by Non-linear Registration of Autofluorescence Images;** Nathan Heath Patterson^{1,2}; Nico Verbeeck³; Raf Van de Plas^{1,3}; Jeffrey Spraggins^{1,4}; Richard M. Caprioli^{1,4,5,6,7}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Biochemistry, Vanderbilt University, Nashville, TN; ³Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Chemistry, Vanderbilt University, Nashville, TN; ⁶Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁷Department of Medicine, Vanderbilt University, Nashville, TN
- WOF pm 03:30 **Automated Approach for Comprehensive Interpretation of Correlated ToF-SIMS and AFM Nanomechanical Data Based on Data Analytics;** Anton V. Ievlev¹; Aleeza Leder Macek¹; Ramakrishnan Kannan¹; Stephen Jesse¹; Mitchel J. Doktycz¹; Scott Retterer¹; Sergei V. Kalinin¹; Olga S. Ovchinnikova¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- WOF pm 03:50 **Optimized Processing Workflow for Improved Information Recovery from Large-scale MSI Data;** Kirill Veselkov¹; Jonathan Sleeman²; Emmanuelle Claude³; Ivan Laponogov¹; Mark Towers³; Robert Tonge³; Jeremy K Nicholson¹; Zoltan Takats¹; James Langridge³; ¹Imperial College London, London, UK; ²Center for Biomedicine and Medical Technology, Mannheim, Germany; ³Waters Corporation, Wilmslow, UK
- WOF pm 04:10 **Big Community Data Analytics for Metabolite Imaging Mass Spectrometry;** Vitaly Kovalev¹; Artem Tarasov¹; Andrew Palmer¹; Katja Ovchinnikova¹; Dominik Fay¹; Theodore Alexandrov¹; ¹EMBL, Heidelberg, Germany. The full list of data contributors to METASPACE is online.

2:30-4:30 pm Wednesday
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Michael MacCoss (University of Washington)
Room 101-106 level 1

- WOG pm 02:30 **Mechanistic Insights and Practical Utility of Highly-Charged Protein Ions on Vacuum Source Mass Spectrometers;** Sarah Trimpin¹; Wen-Jing Zhang¹; I-Chung Lu¹; Efsthios Elia¹; Tarick J. El-Baba¹; Corinne A. Lutomski¹; Joshua L. Fischer¹; Ellen D. Inutan^{1,2}; Casey D. Foley¹; Steffen M. Weidner³; ¹Department of Chemistry, Wayne State



WEDNESDAY AFTERNOON ORAL SESSIONS

- WOG pm 02:50 **University, Detroit, MI; ²MSTM, LLC, Newark, DE; ³BAM-Federal Institute for Materials Research and Testing, Berlin, Germany**
Supercharging of Analytes via a Novel Modified Ion Source; Christopher Andrew Wootton¹; Haytham E. M. Hussein¹; Cookson K. C. Chui¹; Mark P Barrow¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, UK
- WOG pm 03:10 **Quantitative Extraction and Ambient Analysis at a Subcellular Level; Julia Laskin¹;** Ruichuan Yin¹; venkateshkumar Prabhakaran¹; Patrick El Khoury¹; ¹Pacific Northwest National Laboratory, Richland, WA
- WOG pm 03:30 **Analytic Directed Screening System for the Rapid Screening of Synthetic Pathways; Michael Wlekiński¹;** Bradley P. Loren¹; Andy Koswara¹; Caitlin E. Falcone¹; Zinia Jaman¹; Kiran Iyer¹; H. Samuel Ewan¹; Christina R. Ferreira¹; Yanyang Hu¹; Kathryn Yamine¹; Adam Hollerbach¹; Tiago JP Sobreira¹; Larisa Avramova¹; David H. Thompson¹; Zoltan K. Nagy¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- WOG pm 03:50 **Microsampling for Proteomic Characterization of Increasingly Smaller Cells in the Vertebrate (Frog) Embryo; Camille Lombard-Banek¹;** Aparna B. Baxi²; Sally A Moody¹; Peter Nemes²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
- WOG pm 04:10 **An Open Port Sampling Interface as a Noncontact Injection System for Coupling Liquid droplet sample Dispensing Systems with Mass spectrometry; Gary J. Van Berkel¹;** Vilmos Kertesz¹; Harry Boeltz²; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²Dispendix GmbH, Stuttgart, Germany

2:30-4:30 pm Wednesday

FUNDAMENTALS: MOLECULAR MODELING AND QUANTUM MECHANICAL CALCULATIONS IN ION MOBILITY AND MS Christopher Chouinard (PNNL) Room 107-110 level 1

- WOH pm 02:30 **Towards Small Molecule Unsupervised Structural Assignment Using TIMS-FT-ICR MS datasets; Paolo Benigni¹;** Francisco Fernandez Lima¹; ¹Florida International University, Miami, FL

- WOH pm 02:50 **Advancements in Traveling Wave Ion Mobility Theory: Assessing the Conformational Heterogeneity of Proteins and Peptides in the Gas Phase; Sugyan M Dixit¹;** Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- WOH pm 03:10 **De novo Elucidation of Protein Structures with Ion Mobility Spectrometry / Mass Spectrometry; Christian Bleiholder¹;** Florida State University, Tallahassee, FL
- WOH pm 03:30 **Integrative Mass Spectrometry Reveals the Conformational States of Protein Supercomplexes: Application to Cullin Ring Ligases in Complex with Cop9 Signalosome; Andy Lau¹;** Zainab Ahdash¹; Chloe Martens¹; Carla Schmidt²; ¹Argyris Politis³; ¹King's College London, London, London; ²Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; ³King's College London, UK
- WOH pm 03:50 **A Coarse-grained Computational Approach to Enable Structure Elucidation of Polymorphic Nucleic Acids by ion Mobility Mass Spectrometry; Rebecca J D'Esposito¹;** Jennifer L Lippens²; Sweta Vangaveti³; Srivathsan Ranganathan³; Dan Fabris¹; ¹University at Albany-SUNY, Albany, NY; ²Amgen, Thousand Oaks, CA; ³The RNA Institute, Albany, NY
- WOH pm 04:10 **Molecular Dynamics Simulations of the Electrospray Process: Why Do Crown Ethers Suppress Protein Supercharging?; Lars Konermann¹;** Haidy Metwally²; ¹Univ. of Western Ontario, London, ON, Canada; ²Univ. of Western Ontario, London, ON, Canada

4:45-5:30 pm Wednesday

ASMS MEETING

Vicki Wysocki, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Sagamore 5-7 level 2

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There are light refreshments in common areas.

01. Career and Collaboration Opportunities in China Presiding: Yinsheng Wang, Andy Tao Room 130

Recent economic development in China has created numerous job opportunities for postdoctoral fellows and graduate students with training in mass spectrometry. The overall objective of this workshop is to provide information to those individuals with interest in seeking job opportunities in China. We plan to invite 6-7 mass spectrometrists from academia, pharmaceutical companies, and instrument vendors in China as panel members for this workshop. These individuals will share with the participating graduate students and postdocs about their experiences and perspectives in finding jobs, establishing an independent research program in universities, hiring mass spectrometrists, and developing international collaborations in China. We believe that the workshop will benefit young and next-generation scientists in mass spectrometry by providing a unique perspective of job opportunities in China and assisting with their career development. The workshop will be mixed with panelist presentations and Q/A session with the participating students and postdocs.

02. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: New Trends Presiding: Francisco Fernandez-Lima, Chistopher Anderton Room 131-132

Recent advances on 2D and 3D Mass Spectrometry analysis has driven many technological advances in biological, biomedical, materials, environmental and forensic sciences. With the development of new and the incorporation of hyphenated techniques during 2D and 3D MS analysis, there is a need to further develop universal, analysis and data processing protocols; definitions; reference guidelines; standard reference materials; and inter-laboratory comparisons. This first workshop will provide an overview of the main 2D and 3D MS technologies from experts in the field and will focus on generating further strategies to integrate existing and new technologies and researches in the area of 2D and 3D MS analysis.

A preliminary list of topics will include:

- High spatial resolution MS analysis (How is defined the spatial for different MS techniques?);
- Applications in Material, Biological and Forensic Sciences;



- iii. 3D MS analysis and depth profiling;
- iv. Theoretical treatment and existing data processing tools (open source and commercial); and
- v. Hyphenated 2D and 3D MS techniques.

The workshop encourages the participation and presentations of new investigators, postdocs and graduate students. A combination of short presentations (2-3 slides/group) from representatives of the 2D and 3D MS techniques, with a balance between academic, national laboratories and industrial researchers will be followed by an open discussion forum. One of the goals of this workshop is to gather researchers and enable the discussion towards the development of an interest group within the ASMS community to address these new scientific challenges.

03. Diversity and Outreach
Presiding: Benjamin Garcia, Rena Robinson
Room 133-134

This workshop will serve as the first open meeting of the ASMS Diversity and Outreach Working Group. At the 2016 ASMS Conference, a committee was assembled and met to outline potential initiatives for enhancing the diversity of our society. Here specifically at this workshop, we will have a series of mini-talks by scientists that besides describing exciting new science, will also focus on their personal journeys into their professional careers. These talks will lead into a Discussion Panel, so that attendees will have a chance to ask any questions to committee members about scientific research paths, career and life choices, applying for next level positions, etc. Lastly, time will also be allotted for discussion of the initiatives of the Diversity and Outreach Working Group, and to solicit feedback from the ASMS community. We hope this workshop will begin to lay down the networking foundations for scientists who are interested in Diversity and Outreach to connect other scientists at all career levels.

04. Galaxy-P in the Cloud: Proteomic Informatics on JetStream
Presiding: Tim Griffin, Pratik Jagtap, Jeremy Fischer
Room 135-136

The Galaxy bioinformatics platform has emerged as a valuable workflow engine for MS-based proteomic informatics. Galaxy enables integration of disparate software tools to build sophisticated workflows for proteomic, and even multi-omic data analysis. An active and collaborative community of researchers, including the Galaxy for proteomics (Galaxy-P) team, continues to extend Galaxy for these applications.

To date, Galaxy-P has been primarily accessible to those who are experienced users of the Galaxy platform. To extend its reach to the greater community, implementation of proteomics software on more accessible and scalable infrastructure is needed.

To address this need, the Galaxy-P team has partnered with the JetStream cyberinfrastructure resource. Maintained at Indiana University and supported by the NSF, Jetstream is a production-level cloud computing resource open to the research community. JetStream supports Galaxy instances as one of its core bioinformatics software.

This workshop will provide participants background on JetStream, including instructions on how it can be accessed and the hardware and software resources available. A hands-on demonstration opportunity will also be provided, highlighting Galaxy-P software and workflows that have been made available on JetStream. Attendees will take away knowledge on how to access this resource and make use of it for their own MS-based proteomics informatics needs.

05. Food Safety & Authenticity: HRMS Applications
(Flavor, Fragrance & Foodstuff Interest Group)
Presiding: David Schroeder, Sara Kern
Room 137-138

Food, Flavor and Fragrance High Resolution Mass Spectrometry (HRMS) applications and developments discussion continuation. Food contaminant, pesticide, non-targeted analyte identification, and natural product authenticity strategies will be discussed.

06. Energy, Petroleum, and Biofuels: Challenges
(Energy Petroleum & Biofuels Interest Group)
Presiding: Mark Barrow, David Stranz
Room 139

Energy-related samples present a number of analytical challenges. Petroleum is a highly complex mixture and mass spectrometry remains at the forefront of methods for sample characterization. Petroleum derivatives, including fuels which include biofuel components, are also areas of growing interest. As a result, researchers are faced with a range of experimental considerations in order to acquire data of high quality. Samples may undergo extraction or separation procedures, such as SARA fractionation, as an initial step. The choice of solvents used during sample preparation and the selection of the ionization method will influence the sample profile. Chromatography and ion mobility may be employed as additional separation approaches, offering potential for structural information while also introducing a further need for optimization. Dynamic range and, for FTMS instruments, space-charge are two of the experimental considerations during data acquisition. With such areas in mind, the workshop will feature discussion of experimental challenges that influence data quality.

07. Undergraduate Research in Mass Spectrometry: Making the Most of It (Undergraduate Research in MS Interest Group)
Presiding: Jim Pesavento, Megan Gessel
Room 140

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.

08. Quantitative Glycomics and Glycoproteomics
Presiding: Yehia Mechref
Room 141-142

The correlations between protein glycosylation and many biological processes and diseases are increasing the demand for quantitative glycomics strategies, enabling sensitive monitoring of changes in the abundance and structure of glycans. This is currently attained through multiple strategies employing several analytical techniques, such as capillary electrophoresis, liquid chromatography, and mass spectrometry. Detection and quantification of glycans often involve labeling with ionic and hydrophobic reagents to enhance detections in spectroscopic and mass spectrometric measurements. Recently, labeling with stable isotopic reagents has also been presented as a very viable strategy enabling relative quantitation. The different strategies available for reliable and sensitive quantitative glycomics will be described and discussed in this workshop, including MS of naïve, permethylated and derivatized glycans. Quantitation through the addition of standards or isotopically labeled glycans will also be discussed. Additionally, quantitative glycomics through stable isotopic labeling will also be discussed, such as stable isotopic labeling by permethylation and reductive amination. Multiplexing quantitative glycomics employing permethylation, TMT reagents, and QUANTITY will be described and discussed.

09. Mass Spectrometry in GMP Environment: Aspects of System Qualification and Method Validation
Presiding: Gyorgy Vas
Room 143-144

The workshop will continue to discuss the aspects of cGMP compliant instrument qualification practices, was started last year. We will discuss recent best practice, industry and regulatory expectations of Mass Spectrometric Instrument Qualification in a cGMP environment. Different solutions will be discussed, how to handle -on a regulatory compliant manner- the lack of regulatory documents and guidance related to this field. This year we will extend the scope for method validation best practice.

Attendees are expected from instrument vendors, pharmaceutical and food industry and regulatory agencies.



**10. Mass Spectrometry in the Developing World:
Supporting Education and Research
Presiding: Kym Faulk
Room 145**

Students in developing nations learn about mass spectrometry from text books. They rarely if ever get to actually see one, and never get to use them. Old but working instruments that are replaced with new versions could be made available to Universities in developing countries to be used for research and teaching purposes. This would entail shipping, installation, training and maintenance which would all require funding and support. Some aspects of maintenance and training could probably be accomplished via Skype and email. The big questions is: Is this feasible? It would be a noble aspiration for ASMS to embrace. It would improve our relations with the developing world and perhaps provide an example for other organizations (e.g. the NMR Society, etc) to follow. The Presider will begin with a brief description of a personal experience that stimulated him to organize this workshop. This was a memorable experience that forged a lifelong and enduring friendship. All those interested are invited to join in a discussion on this topic.

**11. Lipidomics Data Processing and Analyses: Software Tools
(Lipids & Lipidomics Interest Group)
Presiding: Todd Mitchell, Eva Duchoslav
Room 231-234**

One of the key issues in lipidomics experiments is the bottleneck created by the large amount of data generated. Growing awareness of this issue has seen many academics and MS vendors develop software dedicated to the processing and analysis of this data. With a rapidly growing choice of both commercial software and freeware it can be difficult deciding what software is best for your experiment. In this workshop a panel of advanced users and software developers will share their experience with a variety of lipid and lipidomics-compatible software platforms, focusing on capabilities, tips and tricks, and answer your questions on the where, when and how of lipid MS data processing tools.

**12. Data Independent Acquisition Strategies for Quantitative Proteomics: The Challenges of Scaling Up to Meet Demand
(Data Independent Acquisition Interest Group)
Presiding: Ben Collins, Isabell Bludau
Room 235-238**

A basic aim of most proteomics studies is to obtain a protein matrix with quantitative values for multiple proteins across various conditions. Data independent acquisition (DIA) has recently emerged as a promising method to generate such matrices with deep proteome coverage (similar to DDA) and consistent detection and quantification across large sample cohorts (comparable to SRM/PRM methods). A growing number research goals in the life sciences explicitly require the analysis of large numbers of samples (e.g. perturbation/drug screens, genetic association analysis, clinical/biomarkers, ...). But how broad and how deep can we go? What challenges are being encountered when attempting to scale-up? This workshop aims to discuss the scalability of DIA based methods with respect to both the number of conditions being simultaneously analyzed and proteome coverage. We will discuss issues associated with scalability broadly in three categories: proteome coverage of the spectral library (only for peptide-centric scoring), error rate control on the level of protein detection, and quantification consistency across large and heterogeneous sample cohorts. The workshop will focus on introducing the most recent concepts addressing these aspects and further aims to discuss and develop ideas to ensure the reporting of high-quality protein quantification matrices.

**13. Nucleic Acid-based Therapeutics: Structure Identification and Bioanalysis (Oligonucleotides and Nucleic Acids Interest Group)
Presiding: Laixin Wang, Sam Wainhaus
Room 239**

Following small molecules and monoclonal antibodies, nucleic acid-based therapeutics have emerged to be the third major drug development engine in the pharmaceutical industry. Starting from

antisense in 1990s, RNAi in 2000s to CRISPR and mRNA in 2010s. The rise of nucleic acid based therapeutics has coincided with an explosion in the understanding of the genetic cause of diseases, and the growing desire for precision medicine. LC-MS/MS and LC-HRAM are playing critical roles in the structure characterization and quantitative analysis of nucleic acid molecules. This workshop will focus on the assay development of sensitive and specific assays for structure identification and bioanalysis of nucleic acid based therapeutics and their metabolites. Selected presentations will demonstrate the challenges and solutions during the method development and sample analysis. The remaining time will be spent discussing the pitfalls and tips and tricks in sample preparation, LC development and MS optimization.

**14. Ion Mobility Spectrometry: Towards Standard Operating Procedures (Ion Mobility MS Interest Group)
Presiding: Stephen Valentine, Valérie Gabelica,
Brian Clowers
Room 240-242**

In contrast to the m/z ratio which depends on the analyte only, ion mobility fundamentally depends upon the interactions of analyte ions with neutral gas molecules. Measuring gas-phase ion mobility, although becoming widespread, is not yet routine. Given the growing user base and range of home-made and commercial instrumentation, there is a need for standard operating procedures (SOPs), reference materials and well-defined performance metrics to ensure the quality and utility of experiments. The ion mobility spectrometry interest group workshop will provide a forum to discuss (1) the core issues for developing SOPs for IMS and (2) the minimum reporting requirements for peer-reviewed publication and data sharing.

**15. Bioanalysis of Biosimilars
(Regulated Bioanalysis Interest Group)
Presiding: Dian Su, Jian Wang, Fabio Garofolo
Room 243-245**

Biosimilars are not exact duplicates of Innovator Biotherapeutics. Hence, the Regulatory Agency requirements for Biosimilars differ from those of small molecules. One important difference is the required evaluation of "similarity" of the Biosimilar compared to the innovator Biotherapeutic. Bioanalysis of Biosimilars is subject to endogenous interference, requiring specific and selective assay to ensure data reliability. The specificity and selectivity of traditional quantification approaches (Ligand Binding Assays - LBA) are dependent on the interaction of critical reagents to the Biotherapeutic. It is possible that the Innovator and the Biosimilar do not have the same binding characteristics towards the assay critical reagents. In this case, two assays with different critical reagents may be needed and the demonstration of biocomparability may be more complicated. LC-MS/MS and more recently HRMS have shown to be a successful technique for the Bioanalysis of Biotherapeutics. Unlike traditional approaches, LC-MS/MS and HRMS assays can be developed for the Bioanalysis of Biosimilars without using critical reagents and therefore only a single assay is needed for both Biosimilar and Innovator comparison. Experts in the field will share their experience in this highly interactive workshop.

**AFTER 8:00 pm
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL**

**From 6:45 am Thursday
CORPORATE BREAKFAST SEMINARS
Convention Center**

*Detailed schedule on page 15.
Pre-registration recommended, space is limited*

**8:30-10:30 am Thursday
INFORMATICS: INNOVATIONS
Dan Spellman (Merck & Co.)
Hall D level 1**

- ThOA am 08:30 **QCCloud: A Cloud-based Quality Control System for the Proteomics Community**; Cristina Chiva¹; Roger Olivella^{1,2}; Eva Borràs^{1,2}; Guadalupe Espadas^{1,2}; Olga Pastor^{1,2}; Amanda Solé^{1,2}; Eduard Sabidó^{1,2}; ¹*Proteomics Unit, Centre de Regulació Genòmica (CRG), Barcelona Institute of Science and Technology (BIST), Dr. Aiguader 88, Barcelona, Spain*; ²*Universitat Pompeu Fabra (UPF), Dr. Aiguader 88, Barcelona, Spain*
- ThOA am 08:50 **Paradigm Change in de novo Identification of Small Molecules: Giant Spectral Trees**; Tim J. Stratton¹; Jakub Mezey²; Alena Bednarikova²; Andrea Belicova²; Jana Semanova²; Robert Mistrik²; ¹*ThermoFisher, San Jose, CA*; ²*HighChem, Bratislava, Slovakia*
- ThOA am 09:10 **Novoquest: Algorithm for de novo Sequencing of Cyclic Peptide Antibiotics Using Tandem Mass Spectrometry**; Bahar Behsaz¹; Hosein Mohimani¹; Pieter C. Dorrestein¹; William Gerwick¹; Pavel Pevzner¹; ¹*University of California, San Diego, La Jolla, CA*
- ThOA am 09:30 **Software for Proteome Dynamics from Metabolic Labeling and LC-MS**; Mahbubur Rahman¹; Takhar Kasumov²; Rovshan Sadygov³; ¹*UTMB, Galveston, TX*; ²*Northeast Ohio Medical University, Rootstown, OH*; ³*University of Texas, Galveston, TX*
- ThOA am 09:50 **Visualizing Flux Between Proteoforms Implicated in Stress Response by Constructing and Quantifying Proteoform Families**; Anthony J. Cesnik¹; Michael R. Shortreed¹; Leah V. Schaffer¹; Brian L. Frey¹; Rachel A. Knoener¹; Mark Scalf¹; Stefan K. Solntsev¹; Lloyd M. Smith¹; ¹*University of Wisconsin Madison, Madison, WI*
- ThOA am 10:10 **PeptideExplorer: A Repository-scale Intuitive Navigation Interface over Millions of Identifications**; Benjamin Pullman¹; Jeremy Carver¹; Mingxun Wang¹; Nuno Bandeira^{1,2}; ¹*Computer Science and Engineering Department, UC San Diego, San Diego, CA*; ²*Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA*

**8:30-10:30 am Thursday
MS IN THE QC LAB**

**Izabella Sokolowska (Janssen Research & Development)
500 Ballroom level 1**

- ThOB am 08:30 **Quantitation of Capsaicinoids by UPLC/MS using Single Quadrupole Mass Spectrometry in the QC Environment**; Jane E. Guido; *Kalsec, Inc., Kalamazoo, MI*
- ThOB am 08:50 **LC Peak Purity Assessment Using a Novel LC-MS Data Processing Approach**; Adrien Nyakas¹; Agron Selami¹; Hannes Patrik Plattner¹; Dirk Bächle¹; ¹*Bachem AG, Bubendorf, Switzerland*
- ThOB am 09:10 **Mass Spectrometry Applications in Medical Cannabis Contamination Testing**; Scott Kuzdzal¹; Bob Clifford¹; Jeff Dahl²; Dan Davis¹; Nicole Lock³; Paul Winkler²; Julie Kowalski⁴; Jason Zitzer⁵; Derek Laine⁵; ¹*Shimadzu Scientific Instr., Columbia,*

MD; ²*Shimadzu Scientific Instruments, Columbia, MD*; ³*Shimadzu Scientific Instruments, Somerset, NJ*; ⁴*Restek Corporation, Bellefonte, PA*; ⁵*Trace Analytics, Spokane, WA*

- ThOB am 09:30 **Adding Mass Spectrometry Capabilities to LC/UV-based Workflows as Part of Lifecycle Management in the Routine Analysis of Small Biotherapeutics**; Ximo Zhang¹; Robert Birdsall¹; Brooke M. Koshel¹; Joe Fredette¹; Min Du¹; Ying Qing Yu¹; ¹*Waters Corporation, Milford, MA*
- ThOB am 09:50 **Development and Validation of a LC-MS Glycosylation Method for Testing of a Monoclonal Antibody Product Containing Two Glycosylation Sites**; Zhirui Lian¹; Angelia Reed-Bogan¹; Eric Adamec¹; Bryan Harmon¹; Haiyan Lu¹; Bereket Yemane¹; Jean Yang¹; Roujian Zhang¹; ¹*Eli Lilly and Company, Indianapolis, IN*
- ThOB am 10:10 **Automated Data Processing for Quality Monitoring of Biotherapeutics by Multi-attribute Methods (MAMs)**; Joe Shambaugh¹; Stefano Gotta²; David Bush¹; Maurizio Bronzetti¹; Cassandra Wigmore²; ¹*Genedata Inc, Lexington, MA*; ²*Genedata AG, Basel, Switzerland*

**8:30-10:30 am Thursday
MEMBRANE PROTEIN MS
Julian Whitelegge (UCLA)
Sagamore 1-3 level 2**

- ThOC am 08:30 **Native MS Reveals Lipid-dependent Dimer Formation for the Eukaryotic Purine symporter UapA**; Euan Pyle¹; Bernadette Byrne²; Argyris Politis³; ¹*Imperial College London and King's College London, London, UK*; ²*Imperial College London, London*; ³*King's College London, London*
- ThOC am 08:50 **Collision Induced Unfolding Reveals the Regiospecific Ligand Binding Behavior of Integral Membrane Translocator Protein (TSPO)**; Sarah Fantin¹; Shuai Niu¹; Jian Liu²; Richard A. Kerr¹; Shelagh M. Ferguson-Miller²; Brandon T. Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Michigan State University, Lansing, MI*
- ThOC am 09:10 **FT-ICR MS as a bona-fide Platform for Multimeric Membrane Protein Characterization**; Jennifer L. Lippens¹; Michael Nshanian²; Pascal F. Egea²; Joseph A. Loo²; Iain D. G. Campuzano¹; ¹*Amgen, Newbury Park, CA*; ²*UCLA, Los Angeles, CA*
- ThOC am 09:30 **Automated Proteoform Elucidation of Chromatographically Resolved Hyper-Modified Intrinsically Disordered Membrane Proteins**; Daniel A. Plymire¹; John R. Corbett^{1,2}; Casey E. Wing¹; William S. Phipps¹; Steven M. Patrie^{1,2}; ¹*University of Texas Southwestern Medical Center, Dallas, TX*; ²*University of Texas at Dallas, Richardson, TX*
- ThOC am 09:50 **Mapping the Orientation and Sites of Neurosteroid Photolabeling in the Ion Channel, Glic Using Top-Down, Middle-Down, and Bottom-Up Mass Spectrometry**; Wayland W. L. Cheng¹; Zi-Wei Chen¹; Melissa M. Budelier¹; Douglas F. Covey¹; Gustav Akk¹; Evers S. Alex¹; ¹*Washington University in St. Louis, Saint Louis, MO*
- ThOC am 10:10 **Studying the Structural Dynamics of the Eukaryotic Neurotransmitter Transporter dDAT by Hydrogen/Deuterium Exchange Mass Spectrometry**; Anne Kathrine Nielsen^{1,2}; Ingvar R. Möller²; Kasper D. Rand²; Claus J. Loland¹; ¹*Department of Neuroscience and Pharmacology, University of Copenhagen, Copenhagen, Denmark*; ²*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*



THURSDAY MORNING ORAL SESSIONS

8:30-10:30 am Thursday NUCLEIC ACIDS AND OLIGONUCLEOTIDES Kym Faulk (UCLA) Sagamore 4 level 2

- ThOD am 08:30 **Advances in LC-MS of Oligonucleotides**; Michael G. Bartlett¹; Babak Basiri²; ¹University of Georgia, Athens, GA; ²University of Georgia, Athens, GA
- ThOD am 08:50 **Analysis of Global RNA Mononucleoside Modifications by nanoLC-MS/MS**; Kevin A. Janssen¹; Ranran Wu¹; Benjamin A. Garcia¹; ¹Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA
- ThOD am 09:10 **Multiplex Analysis of Oligonucleotides and RNA Digestion Products through polyA Polymerase (PAP) with Azido-Modified NTP Labeling**; Kayla Borland¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- ThOD am 09:30 **System Wide Elucidation of the Dynamics of Proteins Associating with Single Messenger RNAs (mRNAs)**; Erica Jacobs¹; Peter C Fridy¹; Michael P Rout¹; Brian T Chait¹; ¹Rockefeller University, New York, NY
- ThOD am 09:50 **Real-time Monitoring of Nucleic Acid Dynamics by ESI-MS Melting Experiments**; Botros Toro¹; Pan T.X. Li¹; Daniele Fabris¹; ¹SUNY at Albany, Albany, NY
- ThOD am 10:10 **Multi-omic Mass Spectrometry Applications: Dozens of tRNA Modifications and an Alternative Genetic Code Control Dormancy and Antibiotic Resistance in Mycobacteria**; Weiling Maggie Cai¹; Yok Hian Chionh¹; Nicholas Davis²; Jennifer Hu²; Thomas Begley³; Peter Dedon^{1,4}; ¹Singapore-MIT Alliance for Research and Technology, Infectious Disease IRG, Singapore, Singapore; ²Massachusetts Institute of Technology, Cambridge, MA; ³SUNY Polytechnic Institute, Albany, NY; ⁴Massachusetts Institute of Technology, Cambridge, MA

8:30-10:30 am Thursday NATIVE MS IN STRUCTURAL BIOLOGY Frank Sobott (University of Antwerp) Sagamore 5-7 level 2

- ThOE am 08:30 **Probing Structure and Capturing Transient Intermediates by Monitoring Reactions of Protein Assemblies in Real Time by High-Resolution Native Mass Spectrometry**; Paul Dominic B. Olinares¹; Virapat Kieuvongngam²; Natalia Orlova³; Julio C Padovan¹; David Jeruzalmi³; Jue Chen²; Brian T Chait¹; ¹Laboratory of Mass Spectrometry and Gaseous Ion Chemistry, The Rockefeller University, New York, NY; ²The Rockefeller University and Howard Hughes Medical Institute, New York, NY; ³Department of Chemistry and Biochemistry, City College of New York, New York, NY
- ThOE am 08:50 **Structural Characterization of Protein-Lipid Complexes Involved in Clathrin-Mediated Endocytosis**; Johannes Heidemann¹; Maria M. Garcia Alai²; Anna Gieras²; Rob Meijers²; Charlotte Uetrecht^{1,3}; ¹Heinrich Pette Institute, Hamburg, Germany; ²EMBL, Hamburg, Germany; ³XFEL GmbH, Hamburg, Germany
- ThOE am 09:10 **The Molecular Clock of Islet Amyloid Polypeptide: from Dimerization to Deamidation**; Yuko P. Y. Lam¹; Christopher A. Wootton¹; Juan Wei¹; Ian Hands-Portman¹; Mark P. Barrow¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, UK
- ThOE am 09:30 **Structural Transitions of Brome Mosaic Virus Tracked by Charge Detection Mass Spectrometry**; Kevin M Bond¹; Irina B Tsvetkova¹;

- Bogdan Dragnea¹; Martin F Jarrold¹; ¹Indiana University Bloomington, Bloomington, IN
- ThOE am 09:50 **Investigation of Protein-Protein Interactions using Surface Induced Dissociation - Mass Spectrometry**; Stacey Nash¹; Florian Busch¹; Kristina Heyn²; Fabian Rupert²; Rainer Merkl²; Reinhard Sterner²; Vicki Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Institute of Biophysics and Physical Biochemistry, University of Regensburg, Regensburg, Germany
- ThOE am 10:10 **Double Mutant Cycles in the Gas Phase: Measuring Inter-protein Pairwise Interaction Energies from a Single Native Mass Spectrum**; Jelena Cveticanin¹; Miri Sokolovski²; Deborah Hayoun¹; Amnon Horovitz²; Michal Sharon¹; ¹Department of Biomolecular Sciences, Weizmann Institute of Science, Rehovot, Israel; ²Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel

8:30-10:30 am Thursday IMAGING: PHARMACEUTICALS, METABOLITES, AND LIPIDS Andreas Römpp (University of Bayreuth) Wabash level 1

- ThOF am 08:30 **A Multimodal Imaging Approach to Characterize Intramuscular and Subcutaneous Drug Depots of Cabotegravir**; Reid Groseclose¹; Fang Xie¹; Beat Jucker¹; Hasan Alsaïd¹; Manish Gupta¹; Stephen Castellino¹; ¹GlaxoSmithKline, King of Prussia, PA
- ThOF am 08:50 **Drug Localization at the Single Cell Level - A Multimodal Mass Spectrometry Imaging Approach**; Neda Najafinobar¹; Lena von Sydow¹; Mike J. Hickey¹; Chad S. Elmore¹; Michael E. Kurczyk¹; Magnus Klarqvist¹; Tineke Papavoine²; Per Malmberg³; ¹Astrazeneca, Mölndal, Mölndal; ²AstraZeneca R&D, Gothenburg, Sweden; ³Chalmers University of Technology, Gothenburg, Sweden
- ThOF am 09:10 **Spatial Single-cell Metabolomics of Monolayer Cell Cultures with 10 um Resolution**; Luca Rappez¹; Bachir El Debs¹; Andrew Palmer¹; Artem Tarasov¹; Vitaly Kovalev¹; Ivan Protsyuk¹; Mira Stadler²; Prasad Phapale¹; Megan Stanifer²; Joel Selkrig¹; Mathias Heikenwälder²; Steeve Boulant²; Nassos Typas¹; Theodore Alexandrov^{1,3}; ¹EMBL, Heidelberg, Heidelberg; ²German Cancer Research Center (DKFZ), Heidelberg, Germany; ³Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA
- ThOF am 09:30 **Characterization of Diet-induced Molecular Changes in Ovarian Reserves of Aedes aegypti Using 3D-MSI-TOF-SIMS and MALDI FT-ICR MS**; Anthony Castellanos¹; Quentin Vanbellingen²; Paolo Benigni²; Veronika Michalkova²; Marcela Nouzova²; Fernando Noriega²; Francisco Fernandez-Lima²; ¹Florida International University, Miami, FL; ²Florida International University, Miami, FL
- ThOF am 09:50 **Molecular Insights of the Song Learning Behaviour of Zebra Finch during Ontogeny with Multimodal Mass Spectrometry Imaging**; Nina Ogrinc Potocnik¹; Julie Hamaide²; Tiffany Porta¹; Garima Yadav²; Arnoud Prop¹; Annemie van der Linden²; Ron MA Heeren¹; ¹M4i Institute, Division of Imaging Mass Spectrometry, Maastricht University, Maastricht, Netherlands; ²Bio-Imaging Lab, University of Antwerp, Wilrijk, Belgium
- ThOF am 10:10 **Three-Dimensional MALDI MSI Reveals Distinct Metabolic Compartments and Unique Metabolite Distributions in Soybean Root Nodules**; Dusan Velickovic¹; Beverly Agtuca²; Sylwia Stopka³;



Akos Vertes³; David W. Koppenaal¹; Ljiljana Pasa-Tolic¹; Gary Stacey²; Christopher R. Anderton¹;
¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Earth and Biological Sciences Directorate, Richland, WA;
²Divisions of Plant Sciences and Biochemistry, C. S. Bond Life Sciences Center, University of Missouri, Columbia, MO; ³Department of Chemistry, W. M. Keck Institute for Proteomics Technology and Applications, The George Washington University, Washington, DC

8:30-10:30 am Thursday
GC/MS, GC/GC/MS, GC/MS/MS, AND GC/HRMS
Tom Doherty (Agilent)
Room 101-106 level 1

- ThOG am 08:30 **Comprehensive Steroid Analysis by GCxGC-TOFMS**; Michael Groessl¹; Andrea Bileck¹; Sofia Verouti¹; Genevieve Escher¹; ¹University Hospital Bern, Bern, Switzerland
- ThOG am 08:50 **Application of Py-GCxGC/MS Combined with Chemometrics for the Elucidation of Ancient East Asian Papermaking Materials**; Bin Han¹; Jérôme Vial²; Masamitsu Inaba³; Michel Sablier¹;
¹Sorbonne Universités, Centre de Recherche sur la Conservation (CRC, USR 3224), Muséum national d'Histoire naturelle, Ministère de la Culture et de la Communication, CNRS, Paris, France; ²Department of Analytical, Bioanalytical Sciences and Miniaturization (LSABM), Institute of Chemistry, Biology and Innovation (CBI)-ESPCI ParisTech, CNRS UMR 8231, Paris, France; ³Conservation Science Laboratory, Graduate School of Conservation, Tokyo Geijutsu Daigaku, Taito-ku, Japan
- ThOG am 09:10 **Shifting the Paradigm in Gas Chromatography Mass Spectrometry Pesticide Analysis by High Resolution Mass Spectrometry**; Samanta Uclés¹; Ana Lozano¹; Francisco José Díaz-Galiano¹; Amadeo R. Fernández-Alba¹; ¹European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, ALMERÍA, Spain
- ThOG am 09:30 **GC-QTOFMS and GC-MS/MS with EI and CI as Highly Versatile Platforms for Metabolomics and Metabolic Flux Analysis in Biotechnology**; Teresa Mairinger^{1,2}; Christina Troyer¹; Wolfhard Wegscheider³; Juergen Zanghellini^{1,2}; Diethard Mattanovich^{1,2}; Gunda Koellensperger⁴; Stephan Hann^{1,2}; ¹BOKU-Vienna, Vienna, Austria; ²Austrian Centre of Industrial Biotechnology, Vienna, Austria; ³Montanuniversität Leoben, Leoben, Austria; ⁴University of Vienna, Vienna, Austria
- ThOG am 09:50 **GC-MS with Cold EI for Improved Sample Identification**; Aviv Amirav¹; Alexander B. Fialkov¹; Uri Keshet¹; Tal Alon¹; ¹Tel Aviv University, Tel Aviv, Israel
- ThOG am 10:10 **Data Quality Assurance Methods for Seized-Drug Mass Spectral Libraries**; Wei Hua Ji¹; William E. Wallace¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD

8:30-10:30 am Thursday
FUNDAMENTALS FOR EVERYONE
Nick Polfer (University of Florida)
Room 107-110 level 1

- ThOH am 08:30 **Mass Resolution, Mass Resolving Power, Mass Accuracy, and Mass Calibration: State of the Art and Future Prospects**; Alan G. Marshall^{1,2}; Lissa C. Anderson¹; Greg T. Blakney³; Yuri E. Corilo³; Ryan P. Rodgers^{3,4}; Donald F. Smith³; Chad R. Weisbrod³;

Christopher L. Hendrickson^{3,4}; ¹Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; ²Dept. of Chemistry & Biochemistry, Florida State University, Tallahassee, FL; ³ICR Program, NHMFL, Tallahassee, FL; ⁴Dept. of Chemistry Biochemistry, Florida State University, Tallahassee, FL

- ThOH am 08:50 **How to Reconstruct Collision Cross Section Distributions from Arrival Time Distributions measured in Drift Tube IMS**; Adrien Marchand¹; Sandrine Livet¹; Solenne Delahaye¹; Frédéric Rosu²; Valérie Gabelica¹; ¹University of Bordeaux, Pessac, FR; ²IECB, Bordeaux, France
- ThOH am 09:10 **Mechanistic Insights Gained from Spontaneous Ionization Using Solid or Solvent Matrices**; Charles N. McEwen^{1,2}; Madeline A. Fenner¹; Khoa Hoang¹; Milan Pophristic²; ¹Univ. of the Sciences, Philadelphia, PA; ²MSTM, LLC., Newark, DE
- ThOH am 09:30 **Can Electrospray Ionization Tolerate High Concentrations (100+ mM) of Nonvolatile Salts?**; Anna C. Susa¹; Zijie Xia¹; Evan R. Williams²; ¹University of California, Berkeley, Berkeley, CA; ²University of California, Berkeley, Berkeley, CA
- ThOH am 09:50 **How Hot are Your Ions Really? Experimental Measurements of the Bond Energies of Benzylpyridinium "Thermometer" Ions**; John E. Carpenter¹; Christopher P. McNary¹; April Furin¹; Andrew Sweeney¹; Peter B. Armentrout¹; ¹University of Utah, Salt Lake City, UT
- ThOH am 10:10 **Making Ions Shine with Mass Spectrometry and UV/vis Spectroscopy: Powerful Potential and Potential Pitfalls**; Rebecca A. Jockusch¹; Sydney M.J. Wellman²; Martin F. Czar²; Stephen V. Sciuto²; ¹University of Toronto, Toronto, ON, Canada; ²University of Toronto, Toronto, ON, Canada

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 INFORMATICS: DISCOVERY PROTEOMICS Masaru Miyagi (Case Western University) Hall D

- ThOA pm 02:30 **The Spectra-Cluster Toolsuite: Enhancing Proteomics Analysis Through Spectrum Clustering**; Johannes Griss^{1,2}; Juan Antonio Vizcaino²; ¹Medical University of Vienna, KIMCL, Vienna, No State/Province; ²EMBL-EBI, Cambridge, Cambridgeshire
- ThOA pm 02:50 **Illuminating the "Dark Matter" of Shotgun Proteomics Using MSFragger**; Andy Kong¹; Dmitry M. Avtonomov¹; Felipe Leprevost¹; Dattatreya Mellacheruvu¹; Alexey Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- ThOA pm 03:10 **Discovery of Fusion Peptides through Bottom-Up Proteomic Analysis Using Separate b and y-Ion Databases**; Zach Rolfs¹; Stefan K. Solntsev¹; Michael R. Shortreed¹; Brian L. Frey¹; Mark Scalf¹; Alan D. Attie¹; Lloyd M. Smith¹; ¹University of Wisconsin-Madison, Madison, WI
- ThOA pm 03:30 **Mango: A General Search Tool for CID-cleavage Cross-linked Peptide Identification**; Jared P. Mohr¹; Poorna Perumalla¹; Juan D. Chavez¹; Jimmy K Eng¹; James E. Bruce¹; ¹University of Washington Genome Sciences, Seattle, WA
- ThOA pm 03:50 **Predicting Kinase-Substrate Associations Using Patterns of Co-Phosphorylation**; Marzieh Ayati¹; Danica Wiredja²; Daniela Schlatter²; Sean Maxwell²; Mehmet Koyuturk^{1,2}; Mark R. Chance²; ¹Case Western Reserve University, Cleveland, OH; ²Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH
- ThOA pm 04:10 **Network Discovery of Chronologically Conserved Proteome Dynamics between the Cells and the Tissues**; Mahbubur Rahman¹; Rovshan Sadygov¹; ¹UTMB, Galveston, TX

2:30-4:30 pm Thursday HRMS FOR QUANTITATION IN DRUG DISCOVERY, DEVELOPMENT AND BEYOND Martha Stapels (Sanofi) 500 Ballroom level 1

- ThOB pm 02:30 **High Mass Analysis and Signal Processing on an FT-ICR: From Native Monoclonal Antibodies to Antibody Drug Conjugates and Beyond**; Iain D. G. Campuzano¹; Steve Van Orden²; Huilin Li³; David Kilgour⁴; Jennifer L Lippens¹; Michael Nshanian³; Chawita Netirojjanakul¹; Piriya Wongkongkathep³; Pascal F Egea³; Joseph A Loo³; ¹Amgen Inc., Thousand Oaks, CA; ²Bruker Daltonic, Billerica, MA; ³University of California, Los Angeles, Los Angeles, CA; ⁴Nottingham Trent University, Nottingham, UK
- ThOB pm 02:50 **Discovery of Sequence Variants during IgG1 Monoclonal Antibody Cell Line Selection by High-throughput LC-MS Analysis**; Yan Wang¹; Chongfeng Xu¹; Zoran Sosic¹; Li Zang¹; ¹Biogen, Cambridge, MA
- ThOB pm 03:10 **Role of Copper Incorporation from CuATSM in the Turnover of SOD1 in ALS Mouse Models**; Joe Beckman¹; Blaine Roberts²; Valery G. Voinov³; Yuri Vasil'ev³; ¹Oregon State University, Corvallis, OR; ²Florey Institute of Neuroscience, Melbourne, Australia; ³e-MSion, Corvallis, OR
- ThOB pm 03:30 **ETD and CID MS/MS Analysis at 21 T and X-Ray Crystallography Define Structural Differences in Variants of 45 kDa Proteins**; Lissa Anderson¹; Maria Håkansson²; Björn Walse²; Carol Nilsson^{3,4}; ¹NHMFL, Tallahassee, FL; ²SARomics Biostructures AB, Lund, Sweden; ³Lund University, Lund, Sweden

- ThOB pm 03:50 **High Resolution Mass Spectrometry towards Targeted Residual CHO Protein Quantification**; Matt Schenauer¹; Doug Rehder¹; Darren Brown¹; ¹Gilead Sciences, Oceanside, CA
- ThOB pm 04:10 **Understanding the Metabolism of the Anticancer Drug Triapine Using Electrochemistry AND Liquid Chromatography Coupled to Mass Spectrometry (EC/LC/MS)**; Karla Pelivan¹; Lisa Frensemeier²; Uwe Karst²; Gunda Koellensperger³; Petra Heffeter⁴; Walter Berger⁴; Christian Kowol¹; Bernhard Keppler¹; ¹Institute of Inorganic Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; ²Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany; ³Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; ⁴Institute of Cancer Research, Medical University of Vienna, Vienna, Austria

2:30-4:30 pm Thursday TOP DOWN PROTEIN ANALYSIS Brandon Rutolo (University of Michigan) Sagamore 1-3 level 2

- ThOC pm 02:30 **Top-Down Mass Spectrometry of Large Proteins up to 223 kDa Enabled by Serial Size Exclusion Chromatography**; Trisha Tucholski¹; Wenxuan Cai¹; Bifan Chen¹; Andrew J Alpert²; Samantha Knott¹; Ying Ge¹; ¹University of Wisconsin, Madison, Madison, WI; ²PolyLC Inc., Columbia, MD
- ThOC pm 02:50 **Autopiquer - New Developments in Robust Peak Picking for Mass Spectra**; David P. A. Kilgour¹; Anton N. Kozhinov²; Konstantin O. Nagornov²; Samantha L. Kilgour³; Manuela Tosin³; Sam Hughes⁴; Colin Logan Mackay⁴; Magnus Palmblad⁵; David J. Clarke⁴; David Boocock¹; Yuri O. Tsybin²; ¹Nottingham Trent University, Nottingham, UK; ²Spectroswiss Sàrl, Lausanne, Switzerland; ³University of Warwick, Coventry, UK; ⁴University of Edinburgh, Edinburgh, UK; ⁵Leiden University Medical Center, Leiden, Netherlands
- ThOC pm 03:10 **Characterization of Surface Induced Dissociation (SID) as a Top-Down Fragmentation Technique**; Alyssa Q. Stiving¹; Joshua D. Gilbert¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- ThOC pm 03:30 **Elucidation of Combinatorial Post Translational Modifications (PTMs) of Histones via Top-Down Analysis Using 193 nm Ultraviolet Photodissociation (UVPD)**; Sylvester Greer¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThOC pm 03:50 **Developments in Instrumentation and Data Acquisition Methods for Top-down 21 T FT-ICR Proteomics**; Lissa C. Anderson¹; Chad R. Weisbrod¹; Nathan K. Kaiser¹; Greg T. Blakney¹; Christopher L. Hendrickson^{1,2}; Alan G. Marshall^{1,2}; ¹Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; ²Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- ThOC pm 04:10 **The Omni-trap: A New Processing Cell Equipped with an Extensive Arsenal of Ion Activation Techniques for Top-down Mass spectrometry**; Dimitris Papanastasiou¹; Diamantis Kounadis²; Alexander Lekkas²; Andreas Bozatzidis²; Ioannis Orfanopoulos²; Emmanuel Raptakis²; Maria Reinhardt-Szyba³; Eugen Damoc³; Alexander Makarov³; Roman Zubarev⁴; ¹Fasmatech, Athens, Attiki; ²Fasmatech Science & Technology, Athens, Greece; ³ThermoFisher, Bremen, Bremen; ⁴Karolinska Institute, Stockholm, Uppland



2:30-4:30 pm Thursday

CARBOHYDRATES

Brad Bendiak (University of Colorado HSC)
Sagamore 4 level 2

- ThOD pm 02:30 **Glycoanalysis with Cold Ion Spectroscopy and Ion Mobility: Study of Glycosaminoglycans and Human Milk Oligosaccharides;** Neelam Khanal¹; Chiara Masellis²; Michael Z. Kamrath²; David E Clemmer¹; Thomas R. Rizzo²; ¹Indiana University, Bloomington, IN; ²EPFL, Lausanne, Switzerland
- ThOD pm 02:50 **Disentangling Carbohydrate Isomer Mixtures via Combination of Metal Ion Binding, Gas-Phase Ion Chemistry, Tandem Mass Spectrometry and Ion Mobility Spectrometry;** Katherine Schumacher¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- ThOD pm 03:10 **Electronic Excitation Dissociation Characterization of Native Glycans Derivatized with a Reducing-End Fixed Charge;** Yang Tang¹; Yi Pu¹; Catherine E. Costello¹; Cheng Lin¹; ¹Boston University, Boston, MA
- ThOD pm 03:30 **Identifying Carbohydrate Isomers via an Ion/Molecule Reaction with Water;** Matthew T. Campbell¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThOD pm 03:50 **An Integrated Capillary Electrophoresis-Mass Spectrometry Platform for the Analysis of Glycosaminoglycan Mixtures;** Patience Sanderson¹; Morgan Stickney²; Franklin E Leach III²; James Xia³; Yanlei Yu⁴; Fuming Zhang⁵; Robert J Linhardt⁴; Jonathan I Amster²; ¹University of Georgia, Athens, GA; ²University of Georgia, Athens, GA; ³CMP Scientific, Corp., Brooklyn, NY; ⁴Rensselaer Polytechnic Institute, Troy, NY; ⁵Rensselaer Polytechnic Institute, Troy, NY
- ThOD pm 04:10 **Cationized Carbohydrate Fragmentation Chemistry: Influence of Glycosidic Linkage Position and Stereochemistry;** Benjamin Bythell¹; Jordan M Rabus¹; Maha T. Abutokaikah¹; ¹University of Missouri-St. Louis, St. Louis, MO

2:30-4:30 pm Thursday

PROTEIN-LIGAND INTERACTIONS

Robert Cole (Johns Hopkins University)
Sagamore 5-7 level 2

- ThOE pm 02:30 **Novel Methodology for Pulldown of RNA-Binding Proteins and Application to let-7 miRNAs;** Lisa Jenkins¹; Genevieve Di Tomasso²; Pascale Legault²; ¹National Cancer Institute, Bethesda, MD; ²Université de Montréal, Montréal, QC, Canada
- ThOE pm 02:50 **Improved Identification of Ligand Binding Sites in Integral Membrane Proteins;** Melissa M Budelier¹; Wayland W.L. Cheng¹; Zi-Wei Chen¹; Douglas F Covey¹; James W Janetka¹; Alex S Evers¹; ¹Washington University, St Louis, MO
- ThOE pm 03:10 **On Chip Interaction Proteomics for Low Input Protein Samples;** Cristina Furlan¹; René A.M. Dirks¹; Peter Thomas²; Robert C. Jones²; Hendrik Marks¹; Michiel Vermeulen¹; ¹Radboud University, Nijmegen; ²Fluidigm Corporation, South San Francisco, CA
- ThOE pm 03:30 **Native Top-Down Mass Spectrometry used for the Characterization of Novel Metal Binding by Endogenous Proteins and Complexes;** Nicole A. Haverland¹; Owen S. Skinner¹; Luca Fornelli¹; Areeba A. Tariq¹; Luis F. Schachner¹; Philip D. Compton¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
- ThOE pm 03:50 **Contributions of Individual Ligands to the Structural Stability of an Iron Binding Protein**

During an Unfolding Transition; Daniel W. Woodall¹; Tarick J. El-Baba¹; Wen Liu²; Yang Liu²; Arthur Laganowsky²; David E. Clemmer¹; ¹Indiana University, Bloomington, IN; ²Texas A&M University, College Station, TX

- ThOE pm 04:10 **Online Monitoring of Enzymatic Reactions Using Time-Resolved Desorption Electrospray Ionization Mass Spectrometry;** Hao Chen¹; Si Cheng¹; Qihua Wu¹; ¹Ohio University, Athens, OH

2:30-4:30 pm Thursday

IMAGING: BIOMEDICAL APPLICATIONS

Troy Wood (SUNY Buffalo)
Wabash level 1

- ThOF pm 02:30 **Tumor Margin Determination during Neurosurgery using DESI;** R. Graham Cooks¹; Valentina Pirro²; Clint Miles Alfaro²; Alan Jarmusch²; Eyas M Hattab³; Aaron A Cohen-Gadol⁴; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN; ³Indiana University, Bloomington, IN; ⁴Indiana University-Purdue University, Indianapolis, IN
- ThOF pm 02:50 **Predicting ER, PR, and HER2 Status in Breast Cancer Using Metabolic Markers by DESI-MS Imaging;** Kyana Garza¹; Raquel Mary Rodrigues Peres²; Andréia M Porcari²; Jialing Zhang¹; Jonathan Young¹; Robert J. Tibshirani³; Geisilene Russano de Paiva²; Wendong Yu⁴; Chandandeep Nagi⁴; Marcos N. Eberlin²; Luis O. Zanatta Sarian²; Livia S. Eberlin¹; ¹University of Texas at Austin, Austin, TX; ²State University of Campinas, Campinas, Brazil; ³Stanford University, Stanford, CA; ⁴Baylor College of Medicine, Houston, TX
- ThOF pm 03:10 **Molecular and Elemental Mass Spectrometry Imaging of Photosensitizers in Human Brain Tumors after Fluorescence-guided Resection;** Sabrina Kröger¹; Ann-Christin Niehoff¹; Astrid Jeibmann²; Walter Stummer³; Uwe Karst¹; ¹University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; ²University Hospital of Münster, Institute of Neuropathology, Münster, Germany; ³University Hospital of Münster, Department of Neurosurgery, Münster, Germany
- ThOF pm 03:30 **Building an Accurate Model of the Invasive Tumor Microenvironment with Colon Carcinoma Three Dimensional Tumor Spheroids;** Eric M. Weaver¹; Pinar Zorlutuna^{1,2}; Amanda B. Hummon^{1,3}; ¹Harper Cancer Research Institute, University of Notre Dame, Notre Dame, IN; ²Department of Aerospace and Mechanical Engineering, Bioengineering Graduate Program University of Notre Dame, Notre Dame, IN; ³Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN
- ThOF pm 03:50 **Mapping Non-alcoholic Fatty Liver Disease Progression with Mass Spectrometry Imaging;** Zoe Hall¹; Nicholas J Bond¹; Tom Ashmore¹; Julian L Griffin¹; ¹Department of Biochemistry, University of Cambridge, Cambridge, UK
- ThOF pm 04:10 **Characterization of Single Fluorescent Motor Neurons in Amyotrophic Lateral Sclerosis (ALS) Mouse Brains via MALDI Mass Spectrometry Imaging (MSI);** Catherine M. Rawlins¹; David Calligaris²; Jared R. Auclair¹; April J. Harry^{1,3}; Kylie A. Bemis¹; Ed Luther¹; Olga Vitek¹; Nathalie Y.R. Agar²; Jeffrey N. Agar¹; ¹Northeastern University, Boston, MA; ²Brigham and Women's Hospital, Harvard Medical School, Boston, MA; ³Purdue University, West Lafayette, IN



THURSDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Thursday

INSTRUMENTATION: INNOVATIVE SEPARATIONS APPROACHES COUPLED TO MS

Mary Wirth (Purdue University)
Room 101-106 level 1

- ThOG pm 02:30 **A Method and a Hyphenated to Mass Spectrometry Device for Isolation, Detection and Quantification of Abnormal Proteoforms in blood;** Roman Zubarev; Karolinska Institute, Stockholm, Uppland
- ThOG pm 02:50 **Discovery Bottom-up Proteomic Characterization for Limited Populations of Neurons by Ultrasensitive CE-nanoESI-MS;** Sam Choi¹; Marta Zamarbide¹; M. Chiara Manzini¹; Peter Nemes²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
- ThOG pm 03:10 **Chip-Based Capillary Electrophoresis Mass Spectrometry (CE/MS) for Rapid Intact Mass and Structure Analysis for Large and Small Molecules;** Tawnya Flick¹; Laura Blue²; Shawn Pope²; J. Scott Mellors³; ¹Amgen Inc., Thousand Oaks, California; ²Amgen, Thousand Oaks, CA; ³908 Devices Inc., Boston, MA
- ThOG pm 03:30 **An MS Based Rapid Alternative to Western Blotting;** Fred Regnier¹; Jinhee Kim²; Christian Vukas²; ¹Purdue University / Novilytic, Carmel, IN; ²Novilytic LLC, West Lafayette, IN
- ThOG pm 03:50 **Accumulation and Compression of Billions of Ions Using CRIMP in SLIM Significantly Improves Sensitivity and Ion Mobility Resolution;** Liulin Deng¹; Sandilya Garimella¹; Ahmed Mohamed Hamid¹; Ian K Webb¹; Xueyun Y Zheng¹; Roza Wojcik¹; Spencer A Prost¹; Gordon A Anderson¹; Erin S Baker¹; Yehia M Ibrahim¹; Richard D. Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA
- ThOG pm 04:10 **Analysis of Proteins, Protein Complexes and Protein-Ligand Interactions using Size Exclusion Chromatography-High Resolution Mass Spectrometry;** Aniruddha Sahasrabudhe¹; Florian Busch¹; Zachary VanAernum¹; Brian Rivera²; Vicki Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Phenomenex, Inc., Torrance, CA

2:30-4:30 pm Thursday

ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND APPLICATIONS

Ryan Rodgers (National High Magnetic Field Lab)
Room 107-110

- ThOH pm 02:30 **High-temperature GC×GC with 70eV EI and 10.5eV SPI Nominal and High-resolution TOFMS for the Characterization of Heavy Petroleum Matrices;** Maximilian Jennerwein^{1,2}; Uwe Kaefer^{2,3}; Ralf Zimmermann^{2,3}; Juergen Wendt⁴; Thomas Wilharm¹; Thomas Groeger³; ¹ASG Analytik Service-Gesellschaft mbH, Neusäss, Germany; ²Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ³Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; ⁴LECO European Application & Technology Centre, Berlin, Germany
- ThOH pm 02:50 **Understanding the Structural Space of Hydrocarbons in Crude Oil Using TIMS-FT-ICR MS;** Paolo Benigni¹; Mark E. Ridgeway²; Melvin A Park²; Francisco Fernandez-Lima^{1,3}; ¹Florida Intl University, Miami, FL; ²Bruker Daltonics, Billerica, MA; ³Biomolecular Sciences Institute, Miami, FL

- ThOH pm 03:10 **Application of Selective Labeling Reactions to Explore Structure of Fossil Humic Substances by FT ICR MS;** Alexander Zherebker^{1,2}; Yury Kostyukevich^{2,3,4}; Alexey S Kononikhin^{2,4,5}; Oleg Kharybin³; Irina V Perminova¹; Eugene (Evgeny) Nikolaev^{2,3,4,5}; ¹Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; ³Skolkovo Institute of Science and Technology, Skolkovo, Russia; ⁴Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; ⁵Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia
- ThOH pm 03:30 **Rapid Characterization of Polyalphaolefins Using Atmospheric Pressure Photoionization and Atmospheric Solid Analysis Probe Coupled to Ion Mobility - Mass Spectrometry;** Anna Luiza Mendes Siqueira^{1,2}; Mathieu Beaumesnil^{1,2}; Corinne Loutelier-Bourhis²; Carlos Afonso²; Amandine Racaud¹; ¹TOTAL Marketing & Services, Research Center, Solaize, France; ²Normandie Univ., UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France
- ThOH pm 03:50 **Composition Analysis of Aviation Fuels and Fuel Additives for Rational Development of Renewable Aviation Fuels;** Katherine Wehde¹; Mark Romanczyk¹; Petr Vozka²; Jorge Ramirez Velasco³; Rodney Trice³; Gozdem Kilaz²; Hilikka Kenttamaa¹; ¹Department of Chemistry, Purdue University, West Lafayette, IN; ²Department of Aviation Technology, Purdue University, West Lafayette, IN; ³Department of Materials Engineering, Purdue University, West Lafayette, IN
- ThOH pm 04:10 **Complementarity of ESI, APPI and LDI FT-ICR MS Analyses for the Comprehensive Description of Raw and Deoxygenated Pyrolysis Bio-oils;** Jasmine Hertzog¹; Vincent Carré¹; Liangyuan Jia²; Yann Le Brech²; Ludovic Pinard³; Colin Logan Mackay⁴; Ondřej Mašek⁵; Anthony Dufour²; Frédéric Aubriet¹; ¹LCP-A2MC - Université de Lorraine, Metz, France; ²LRGP - Université de Lorraine, Nancy, France; ³IC2MP - Université de Poitiers, Poitiers, France; ⁴School of Chemistry - University of Edinburgh, Edinburgh, UK; ⁵UK Biochar Research Center - University of Edinburgh, Edinburgh, UK

4:45-5:30 pm Thursday

PLENARY LECTURE

Richard A. Yost (University of Florida)
Hall D level 1



Saving the Great Coral Reefs

Kristen Marhaver
Research Station Carnabi

6:30-9:00 pm Thursday

CLOSING EVENT

INDIANA STATE MUSEUM

Advance purchase ticket is required (\$30).

POSTER OVERVIEW



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

Ambient Ionization: Fundamentals and Instrumentation	001 - 016
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Biomarkers: Discovery I.....	028 - 050
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling I.....	051 - 071
Carbohydrates I.....	072 - 098
Clinical Analysis I.....	099 - 119
Drug Discovery/DMPK/ADME.....	120 - 150
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Energy: Hydrocarbon and Petrochemical.....	158 - 181
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Forensics I.....	213 - 232
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Fundamentals: Metal Ion Cationization, Metal-Ligand Interactions, Catalysis.....	240 - 249
Fundamentals: Photodissociation.....	250 - 253
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Imaging MS: Disease Markers.....	275 - 309
Informatics: Peptide ID and Quantification.....	310 - 341
Instrumentation: New Developments in Ionization and Sampling I.....	342 - 363
Ion Mobility: Applications I.....	364 - 389
LC/MS: Sample Preparation I.....	390 - 405
Lipids: Profile Analysis I.....	406 - 431
Metabolomics: General.....	432 - 463
Metabolomics: Sample Preparation.....	464 - 474
Metabolomics: Targeted and Quantitative Analysis I.....	475 - 495
Metabolomics: Untargeted Metabolite Profiling I.....	496 - 519
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Proteins: Complexes/Non-covalent Interactions I.....	562 - 592
Proteomics: New Approaches.....	593 - 632
Proteomics: Quantitative I.....	633 - 652
Proteomics: Top Down Analysis I.....	653 - 665
Small Molecules: Quantitative Analysis I.....	666 - 689
Systems Biology I.....	690 - 706
Toxicology.....	707 - 721

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

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Informatics: Protein ID and Quantification.....	370 - 378
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Instrumentation: New Developments in Ionization and Sampling II.....	402 - 434
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Metabolomics: Untargeted Metabolite Profiling II.....	504 - 527
Nanomaterials.....	528 - 536
Nucleic Acids and Oligonucleotides I.....	537 - 556
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Proteins: PTMs.....	569 - 601
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Proteomics: Top Down Analysis II.....	653 - 679
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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

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Epigenetic Modifications.....	149 - 161
Exposomics Methodologies and Research Results.....	162 - 163
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Imaging MS: Computational Methods and Analysis.....	275 - 280
Imaging MS: Instrumentation.....	281 - 291
Imaging MS: Sample Preparation.....	292 - 306
Imaging MS: Software.....	307 - 312
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Informatics: Metabolomics.....	323 - 335
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Instrumentation: New Concepts.....	346 - 366
Ion Mobility: Applications II.....	367 - 392
Isotope Labeling and Fluxomics Applications.....	393 - 403
Lipids: ID and Structural Analysis.....	404 - 422
MALDI: Fundamentals and Instrumentation.....	423 - 429
Metabolomics: Clinical Applications.....	430 - 446
Metabolomics: Identification of Unknown Metabolites.....	447 - 465
Metabolomics: Targeted and Quantitative Analysis II.....	466 - 483
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Nanoscale and Microfluidic Separations and MS.....	513 - 522
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Nucleic Acids and Oligonucleotides II.....	543 - 563
Peptides: Sequence Analysis.....	564 - 575
Peptides: Targeted and Quantitative Analysis II.....	576 - 594
Phosphopeptides: Enrichment Methods.....	595 - 603
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Protein Therapeutics: Quantitative Analysis.....	626 - 662
Proteomics: Infectious Diseases.....	663 - 676
Proteomics: Intact Proteins.....	677 - 686
Proteomics: Quantitative III.....	687 - 706
Systems Biology II.....	707 - 719

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

Biomarkers: Discovery II.....	001 - 024
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Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling II.....	052 - 072
Clinical Analysis II.....	073 - 103
Disease Biomarkers.....	105 - 131
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Environmental: General II.....	144 - 175
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions.....	176 - 201
H/D Exchange: Protein Structure/Function.....	202 - 228
High Mass Accuracy/High Performance MS: Applications and Instrumentation.....	229 - 255
Imaging MS: Method Development.....	256 - 286
Imaging MS: Pharmaceutical Applications.....	287 - 306
Informatics: Algorithms and Statistical Advances.....	307 - 336
Informatics: Workflow and Data Management.....	337 - 352
Instrumentation: New Developments in Ion Detection.....	353 - 387
Ion Mobility: FAIMS/DMS.....	388 - 398
Ion Mobility: Fundamentals.....	399 - 422
LC/MS: Chromatography and Software.....	423 - 441
Lipids: Profile Analysis II.....	442 - 453
Lipids: Targeted and Quantitative Analysis.....	454 - 474
MALDI: Applications.....	475 - 491
Metabolomics: Untargeted Metabolite Profiling III.....	492 - 514
Peptides: Fragmentation Mechanisms.....	515 - 518
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Phosphopeptides: Quantitative Analysis.....	552 - 569
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Proteins: Complexes/Non-covalent Interactions II.....	606 - 628
Proteins: Conformation Analysis and Structural Biology.....	629 - 648
Proteomics: Clinical Applications.....	649 - 680
Proteomics: Tissue.....	681 - 698
Small Molecules: Quantitative Analysis III.....	699 - 722



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Ambient Ionization: Fundamentals and Instrumentation	001 - 016
Antibodies & Antibody Drug Conjugates I.....	017 - 027
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Proteomics: New Approaches.....	593 - 632
Proteomics: Quantitative I.....	633 - 652
Proteomics: Top Down Analysis I.....	653 - 665
Small Molecules: Quantitative Analysis I.....	666 - 689
Systems Biology I.....	690 - 706
Toxicology.....	707 - 721

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION 001 - 016

- MP 001 **Exploration of Mixed-gas Flowing Atmospheric-Pressure Afterglow as an Atmospheric Pressure Chemical Ionization and Photoionization Source for Mass Spectrometry;** Sunil Badal¹; Jessica Hellinger¹; Jacob Shelley¹; ¹Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY
- MP 002 **In-vivo Endoscopic Mass Spectrometry with Moving String as Sampling Probe;** Lee Chuin Chen; University of Yamanashi, Kofu, Yamanashi
- MP 003 **Multi-mode Reactive Nano-electrospray Ion Source for Droplet Chemistry using Picoliter Samples;** Dmytro Kulyk¹; Abraham K. Badu-Tawiah²; ¹The Ohio State University, Columbus, Ohio; ²The Ohio State University, Columbus, OH
- MP 004 **Ambient Nanoparticle and Plasma Assisted Laser Desorption Ionization Mass Spectrometric Methods (Ambient nanoPALDI MS) for Live Tissue Analysis;** Jae Young Kim¹; Eun Seok Seo¹; Hyunmin Kim²; Dong-Kwon Lim³; Dae Won Moon¹; ¹Department of New Biology, DGIST, Daegu, South Korea; ²Division of Nano and Energy Convergence Research, DGIST, Daegu, South Korea; ³KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea

- MP 005 **Ambient Chemical Analysis of Biological Tissues by the Combination of Extractive Electrospray Ionization Mass Spectrometry with High-Frequency Resonance Field Desorption;** Vladimir Frankevich¹; Vitaliy V Chagovets¹; Xinchun Wang²; Alisa Tokareva¹; Alexey S Kononikhin¹; Konstantin Chingin²; Huanwen Chen²; Gennady Sukhikh¹; ¹Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, Russia; ²Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China University of Technology, Nanchang, China
- MP 006 **Innovations in Liquid Microjunction Surface Sampling Probe Mass Spectrometry;** Louis Searcy¹; Arun Wanchoo²; Cuong Nguyen²; Timothy J. Garrett²; Richard A Yost²; ¹University of Florida, Gainesville, FL; ²University of Florida, Gainesville, FL
- MP 007 **Multimodal Imaging Combining Fluorescence Microscopy and Laser Ablation Electrospray Ionization Mass Spectrometry;** Sylvia A Stopka¹; Beverly J Agtuca²; Christopher R Anderton³; Rikkita Khattar¹; David W Koppenaal³; Ljiljana Pasa-Tolic³; Gary Stacey²; Akos Vertes¹; ¹George Washington University, Washington, DC; ²University of Missouri, Columbia, MO; ³Pacific Northwest National Laboratory, Richland, WA
- MP 008 **Development of a Continuous Flow Infrared MALDESI Source for Online LC/MS Analysis of Peptides and Proteins;** Koichi Kimura¹; Hisanao Hazama¹; Kunio Awazu^{1,2,3}; ¹Graduate School of Engineering, Suita, Japan; ²Graduate School of Frontier Biosciences, Suita, Japan; ³Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan
- MP 009 **Analytical Validation of a Portable MS System Featuring Interchangeable, Ambient Ionization Sources during Field Operation;** Shahnaz Mukta¹; Zachary E. Lawton¹; William L. Fantigante¹; Herbert Oberacher²; Christopher C. Mulligan¹; ¹Illinois State University, Normal, IL; ²Innsbruck Medical University, Innsbruck, Austria
- MP 010 **Compact Laser Ablation Microwave Plasma Ionization for Ambient Molecular and Atomic Analysis;** Gaston D. Merideth II¹; Kelsey R. May¹; Kenyon Evans-Nguyen¹; ¹The University of Tampa, Tampa, FL
- MP 011 **Novel Ambient Ionization Source for Real-Time Breath Analysis;** Michael Wei¹; Christopher Gongar¹; Michael Costanzo²; Jared Boock³; Richard A. Yost¹; ¹University of Florida, Gainesville, FL; ²Breathtec Biomedical, Inc., Gainesville, Florida; ³Cannabix Technologies, Gainesville, FL
- MP 012 **Theta Emitters for Fast Mixing: Hydrogen-Deuterium Exchange, Ion Form;** Zijie Xia¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- MP 013 **Coated Blade Spray: Shifting the Paradigm of Direct Sample Introduction to Mass Spectrometry;** German Augusto Gomez-Rios¹; Marcos Tascon¹; Nathaly Reyes Garces¹; Daniel Rickert¹; Ezel Boyaci¹; Justen J Poole¹; Karol Jaroch²; Barbara Bojko^{1,2}; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, Ontario; ²Nicolaus Copernicus University in Torun, Bydgoszcz, Poland
- MP 014 **Molecularly Imprinted Membrane Electrospray Ionization for Direct Sample Analyses;** Mei Zhang; Chinese CDC, Beijing, China
- MP 015 **Comparison of the Novel UniSpray Ion Source to A Range of Alternative Atmospheric Pressure Ionization Sources;** Eleanor Riches¹; G. John Langley²; Julie M. Herniman²; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; ²Faculty of Natural and Environmental Sciences, Chemistry, University of Southampton, Highfield, UK



MP 016 **Development and Testing of a Simple, Low-Cost Low-Temperature Plasma Ionization Source;** Clinton A. L. McFeely¹; Victoria Zelikson¹; Scott Gronert¹; ¹Virginia Commonwealth University, Richmond, VA

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
017 - 027

- MP 017 **Accurate Mass Determination of Intact Monoclonal Antibody Charge Variants, Including Deamidation Products, using CZE-CZE-QqTOF-MS;** Kevin Joo^{1,2}; Jens Hühner^{1,3}; Christian Neusüß¹; ¹Aalen University of Applied Sciences, Aalen, Germany; ²Helmholtz Zentrum München, Neuherberg, Germany; ³University of Tübingen, Tübingen, Germany
- MP 018 **Robust and Sensitive Workflow for Qualitative and Quantitative Analysis of Intact Monoclonal Antibodies Using Microflow LC and TripleTOF Mass Spectrometry;** Gavin Fischer; Redwood City
- MP 019 **Analysis of Bispecific mAb by Size Exclusion Chromatography and Mass Spectrometry ;** Keegan Gike¹; Atis Chakrabarti¹; ¹Tosoh Bioscience LLC, King of Prussia, PA
- MP 020 **Charge Heterogeneity Analysis of Intact Monoclonal Antibodies using CESI-MS;** Esme Candish¹; Christopher Loessner²; Stephen J. Lock³; Olga Friese⁴; Elaine Stephens⁵; Jason C. Rouse⁶; Bryan Fonslow¹; ¹SCIEX, Brea, CA; ²SCIEX, Darmstadt, Germany; ³SCIEX, Warrington, UK; ⁴Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; ⁵Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MA
- MP 021 **Manipulation of Chromatographic Conditions to Maximize the LC/MS Effectiveness;** Suresh Babu Cv¹; Ning Tang²; Anne Blackwell³; ¹Agilent Technologies, Bangalore, Karnataka; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Wilmington, DE
- MP 022 **A Quick and Simple Approach for Confirmation of Isomerization and Racemization of Aspartate in Asp-Asp Motifs of a Therapeutic Protein;** Weitao Jia¹; Xiaoxiao Liu¹; Jennifer Zhang¹; ¹Genentech, Inc, South San Francisco, CA
- MP 023 **High-throughput Mass Spectrometric Analysis: From Covalently Labeled Proteins to Antibody Drug Conjugates;** Chawita Netirojjanakul¹; Iain D. G. Campuzano¹; Tisha San Miguel¹; Aiko Umeda¹; Jason Long¹; ¹Amgen, Thousand Oaks, CA
- MP 024 **High Resolution LC/MS Separation and Characterization of Chemoenzymatic Site-specific Engineered Antibody-Drug Conjugates (ADCs);** Shanhua Lin¹; Terry Zhang²; Brian Agnew³; Jonathan Joseph²; Xiaodong Liu⁴; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Eugene, OR; ⁴Thermo Fisher Scientific, Sunnyvale, CA
- MP 025 **Development of a High-Throughput Workflow to Characterize Bispecific Antibody Variants;** Michael Bacica¹; Yaqiong Lin¹; Jing Zhuo¹; Marissa M Horn¹; Karen J Froning¹; Jonathan Fittchett¹; Bryan E. Jones¹; ¹Lilly Research Labs, San Diego, CA
- MP 026 **Characterization of Monoclonal Antibodies and Antibody Drug Conjugates using Microfluidic CE-MS Technology;** Erin Redman¹; Joshua P. Guerrette¹; Michael P. Goodwin²; J. Scott Mellors¹; ¹908 Devices, Inc., Carrboro, NC; ²908 Devices Inc., Boston, MA
- MP 027 **A Novel Capillary Isoelectric Focusing - Mass Spectrometry (cIEF-MS) Technique for Monoclonal Antibody Charge Variants Analysis;** Jun Dai¹; Yingru Zhang²; Fahim Sarah Zarrin³; Rena Wang³; James Xia³; Wayne Heacock⁴; Dat Phan⁴; Dawn Stickle⁴; John Sausen⁴; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Princeton, NJ; ³CMP Scientific, Corp., Brooklyn, N.Y.; ⁴Agilent Technologies, Inc., Wilmington, DE

BIOMARKERS: DISCOVERY I
028 - 050

- MP 028 **Tumor Specific Signature Pathway Showing Differentially Expressed Proteins in Prostate Cell Lines using Proteomics Approach;** Arum Park¹; Jiyeong Lee²; Sora Mun¹; Doo Jin Kim²; Byung Heun Cha²; YuRim Lee⁴; Tag Keun Yoo³; Hee-Gyoo Kang^{1,2}; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam, South Korea; ²Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam, South Korea; ³Department of Urology, College of Medicine, Eulji University, Daejeon, South Korea; ⁴Eulji University, Seongnam-si, South Korea
- MP 029 **Rheumatoid Factor-Correlated Proteins are Useful Screening Markers for Autoimmune and Infectious Diseases with Rheumatoid Factor;** Sora Mun¹; Doojin Kim²; Jiyeong Lee²; Arum Park¹; AeEun Seok¹; Yeon-Tae Chun²; Hee-Gyoo Kang^{1,2}; ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, South Korea; ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea
- MP 030 **Disease-specific IgG Fc N-glycosylations Personalized Biomarkers to Differentiate Lung Cancer from Benign Lung Diseases;** Dan Zhang¹; Tianjing Chen¹; Mo Zhang¹; Zhili Li¹; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing
- MP 031 **Deep Proteome Profiling of Extracellular Vesicles Isolated from Human Plasma;** Ole Østergaard^{1,2}; Christian D. Kelstrup²; Julia T. Tanassi¹; Niels H. H. Heegaard^{1,3}; Jesper V. Olsen²; ¹Statens Serum Institut, Copenhagen, Denmark; ²Novo Nordisk Foundation Center for Protein Research, Faculty of Health Sciences, University of Copenhagen, Copenhagen, Denmark; ³Department of Clinical Biochemistry and Pharmacology, Odense University Hospital, Odense, Denmark
- MP 032 **Collagen Proteins in Colorectal Liver Metastasis;** Nick A. van Huizen¹; Robert R.J. Coebergh van den Braak¹; Michael Doukas¹; Lennard J.M. Dekker¹; Theo M. Luiders¹; Jan N.M. IJzermans¹; ¹Erasmus MC, Rotterdam, Zuid-Holland
- MP 033 **Abundant Protein Depletion of Human Plasma Samples – A Reproducibility and Scaling Study;** Sergei Snovidia¹; Katherine E. Herting²; Ramesh Ganapathy²; Ryan Bomgardner²; Barbara J. Kaboord²; Chris Etienne²; John C. Rogers²; ¹Thermo Fisher Scientific, Rockford, IL; ²ThermoFisher Scientific, Rockford, IL
- MP 034 **Assessment of Neopterin as a Potential Biomarker of Beta Cell Function in Human Urine Utilizing UPLC-MS/MS;** Kimberly A Navetta¹; Jennifer Colangelo²; ¹Pfizer Inc., Groton, CT; ²Pfizer Inc, Groton, CT
- MP 035 **Proteomic Characterization of Laser Microdissected Myometrium and Trophoblast Compartments in Placenta Accreta;** Brian L. Hood¹; Rebecca A. Keller²; Guisong Wang¹; Julie Oliver¹; Melinda M. Sanders³; Xiaohong Wang³; Alfred Khoury⁴; William A. Campbell²; Chad A. Hamilton^{1,5}; George L. Maxwell^{1,4,6}; Thomas P. Conrads^{1,6}; ¹Women's Health Integrated Research Center, Gynecologic Cancer Center of Excellence, Annandale, VA; ²Division of Maternal-Fetal Medicine, Department of Obstetrics & Gynecology, University of Connecticut School of Medicine, Farmington, CT; ³Department of Pathology and Histology, University of Connecticut School of Medicine, Farmington, CT; ⁴Department of Obstetrics & Gynecology, Inova Fairfax Hospital, Falls Church, VA; ⁵Gynecologic Oncology Service, Walter Reed National Military Medical Center, Bethesda, MD; ⁶Inova Schar Cancer Institute, Falls Church, VA



- MP 036 **Dramatic Alterations in RNA Binding and Exosome-Associated Proteins Occur in Breast Cancer as Revealed by Proteomic Analysis of FFPE tissue;** Ten-Yang Yen¹; Moe Thein¹; Roger Yen¹; Bruce A. Macher¹; Leslie C. Timpe¹; ¹*San Francisco State University, San Francisco, CA*
- MP 037 **Identification of Peptides from Dehalococcoides mccartyi Protein Biomarkers in Chloroethene Contaminated Groundwater Samples through a Standard-Free LC-MRM-MS Approach;** Manuel Villalobos^{1,2}; Cynthia M. Swift^{1,2}; Karuna Chourey²; Frank Löffler¹; Robert L. Hettich^{1,2}; ¹*University of Tennessee, Knoxville, TN*; ²*Oak Ridge National Lab, Oak Ridge, TN*
- MP 038 **Lipidomic Analysis of CSF from Patients with Neoplastic Meningitis (NM): A Pilot Study Identifying Biomarkers for Early Detection of NM;** Shinji K. Strain¹; Morris D. Groves²; Mark R. Emmett^{1,3,4,5,6}; ¹*Department of Neuroscience and Cell Biology, University of Texas Medical Branch, Galveston, TX*; ²*Austin Brain Tumor Center, Texas Oncology/US Oncology Research, Austin, TX*; ³*Department of Biochemistry and Molecular Biology, University of Texas Medical Branch, Galveston, TX*; ⁴*Department of Pharmacology and Toxicology, University of Texas Medical Branch, Galveston, TX*; ⁵*Department of Radiation Oncology, University of Texas Medical Branch, Galveston, TX*; ⁶*UTMB Cancer Center, Galveston, TX*
- MP 039 **Epidermal Lipids Detected by Multiple Reaction Monitoring (MRM)-profiling as Potential Biomarkers for Atopic Dermatitis;** Jackeline Franco¹; Christina R. Ferreira²; Tiago José Paschoal Sobreira²; John P. Sundberg³; Harm HogenEsch⁴; ¹*Purdue University, West Lafayette, IN*; ²*Bindley Bioscience Center, Purdue University, West Lafayette, IN*; ³*The Jackson Laboratory, Bar Harbor, MN*; ⁴*Purdue University, West Lafayette, IN*
- MP 040 **Reproducible Single Shot Plasma Proteome Profiling with High Throughput Capabilities on a Robust Capillary Flow Setup;** Roland Bruderer¹; Oliver M. Bernhardt¹; Tejas Gandhi¹; Sebastian Mueller¹; Polina Mironova²; Ondine Walter²; Jérôme Carayol²; Jörg Hager²; Armand Valsesia²; Loïc Dayon²; Jan Muntel¹; Arne Astrup³; Wim H.R. Saris⁴; Lukas Reiter¹; ¹*Biognosys, Zurich, Switzerland*; ²*Nestlé Institute of Health Sciences, Lausanne, Switzerland*; ³*University of Copenhagen, Copenhagen, Denmark*; ⁴*Maastricht University Medical Centre, Maastricht, Netherlands*
- MP 041 **Identification of Predictive Biomarkers of Doxorubicin-induced Clinical Cardiotoxicity;** Li-Rong Yu¹; Jaclyn R. Daniels¹; Zhijun Cao¹; Jinchun Sun¹; Richard D. Beger¹; Issam Makhoul²; Suzanne Klimberg²; Jeanne Wei²; Valentina K. Todorova²; ¹*National Center for Toxicological Research, FDA, Jefferson, AR*; ²*University of Arkansas for Medical Sciences, Little Rock, AR*
- MP 042 **Assessment of the Effects of Pollutants in the Great Lakes on the Human Proteome;** Emmalyn Dupree¹; Bernard Crimmins²; Thomas Holsen²; James Pagano³; Brooke Thompson⁴; Krista Christensen⁴; Michelle Raymond⁴; Costel C. Darie⁵; ¹*Biochemistry and Proteomics Group, Department of Chemistry and Biomolecular Science, Clarkson University, Potsdam, NY*; ²*Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY*; ³*Department of Chemistry, SUNY Oswego, Oswego, NY*; ⁴*Wisconsin Department of Health Services, Madison, WI*; ⁵*Biochemistry & Proteomics Group, Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY*
- MP 043 **Development of a Mass Spectrometry-Based Targeted Quantitative Assay for use in the Identification of a Colorectal Cancer Peptide Signature;** Jia You¹; Athit Kao¹; Roslyn Dillon¹; Lisa J. Croner¹; John E. Blume¹; Ryan W. Benz¹; Bruce E. Wilcox¹; ¹*Applied Proteomics Inc., San Diego, CA*
- MP 044 **Nitroproteome Analysis of a Model of Acute Kidney Injury from Renal Ischemia/Reperfusion;** Pamella Araujo Malagrino¹; Gabriela Venturini²; Rafael Darioli²; Kallyandra Padilha²; Tamiris Gois²; Karina Moraes Cardozo³; Valdemir Melechco Carvalho³; Jessica Silva Salgueiro³; Jose Eduardo Krieger²; Alexandre Costa Pereira²; ¹*São Paulo, São Paulo*; ²*Heart Institute, Sao Paulo, SP*; ³*Fleury Group, Sao Paulo, Brazil*
- MP 045 **In-quest of Biomarkers for Early Diagnosis of Alzheimer's Disease using LC-QTOF-MS/MS Based Lipidomics;** Chandana Mannem¹; Jagan A. Pillai²; Christine Reece²; Yan Xu^{1,3}; ¹*Department of Chemistry, Cleveland State University, Cleveland, OH*; ²*Luo Ruvo Center for Brain Health, Cleveland Clinic, Cleveland, OH*; ³*Case Comprehensive Cancer Center, Case Western Reserve University, Cleveland, OH*
- MP 046 **A Study of Label-Free and Isobaric Tag Approaches for the Detection of Biologically Relevant Changes in PAX8 Overexpressed MOSE Cells;** Melissa R Pergande¹; Laura R Hardy¹; Carol Haney-Ball²; Vadiraja Bhat³; Joanna E. Burdette¹; Stephanie M. Cologna¹; ¹*University of Illinois at Chicago, Chicago, IL*; ²*Agilent Technologies, Inc., Santa Clara, CA*; ³*Agilent Technologies, Inc., Wilmington, DE*
- MP 047 **Use of Phosphoproteomics in Human Induced Pluripotent Stem Cell-Derived Cardiomyocytes for Investigation of Cardiac Toxicity of HCV-NS5B Antiviral Drugs;** Zhenlian Ke Tracy¹; John Imredy¹; Edward Lis¹; Bharathi Balasubramanian¹; Raymond Gonzalez¹; ¹*Merck & Co., West Point, PA*
- MP 048 **Use of Tyr-kinase Inhibitors to Identify Cross-Talk between Signaling Pathways and Novel Protein Drug-Targets;** Iulia M. Lazar¹; Nicole Smith¹; ¹*Virginia Polytechnic Institute & State University, Blacksburg, VA*
- MP 049 **Temporal Effects of Novel Combinatorial Chemotherapeutics on Pancreatic Cancer Cells Investigated via Large-scale, Ion-Current Based Quantitative Proteomics;** Xue Wang^{1,2}; Jin Niu¹; Jun Li¹; Xiaomeng Shen³; Shichen Shen¹; Robert M. Straubinger^{1,2}; Jun Qu^{1,2}; ¹*University at Buffalo, Buffalo, NY*; ²*Roswell Park Cancer Institute, Buffalo, NY*; ³*Amgen, South San Francisco, CA*
- MP 050 **Dried Matrix Spots Sampling in LC-MS Based Non-Targeted Proteomics – What Can You Expect from Different Sampling Materials and Devices?;** Cecilie Rosting¹; Astrid Gjelstad¹; Trine Grønhaug Halvorsen¹; ¹*School of Pharmacy, University of Oslo, Oslo, Norway*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING I 051 - 071

- MP 051 **Proteome-wide Identification of Protein-Protein Interactions by in-vivo Chemical Crosslinking and Mass Spectrometry;** Elena L. Rudashevskaya¹; Tomáš Ječmen¹; Karl A.T. Makepeace^{2,3}; Jason J. Serpa²; Yassene Mohammed^{2,4}; Evgeniy V. Petrotchenko²; Chris Meisinger⁵; Rene Zahedi¹; Albert Sickmann¹; Christoph H. Borchers^{1,2,3}; ¹*Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany*; ²*University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada*; ³*Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*; ⁴*Center for Proteomics and Metabolomics, Leiden University, Netherlands*; ⁵*Institute for Biochemistry and Molecular Biology, Freiburg, Germany*
- MP 052 **Drug Induced Protein Conformational and Interaction Dynamics by Quantitative Cross-linking Mass Spectrometry;** Juan D Chavez¹; Devin K. Schweppe¹; Xuefei Zhong¹; Jimmy K. Eng¹; James E. Bruce¹; ¹*University of Washington, Seattle, WA*



MONDAY POSTERS

- MP 053 **Circularization of Calmodulin by Disulfide Bond: Structural Characterization by LC-MS/MS and Effects on Protein Dynamics by Isothermo Titration Calorimetry;** You-Jun Fu¹; Priya Katyal¹; ¹University of Connecticut, Storrs, CT
- MP 054 **Application of Fast Photochemical Oxidation of Proteins for *in vivo* Modification in *Caenorhabditis elegans*;** Lisa Jones¹; Jessica A Espino¹; ¹University of Maryland, Baltimore, MD
- MP 055 **Dynamics of the Pre-amyloid Structural Change of β -2-microglobulin Studied by Covalent Labeling and Mass Spectrometry;** Blaise G Arden¹; Nicholas B Borotto¹; Brittney Burant¹; Richard W Vachet¹; ¹University of Massachusetts-Amherst, Amherst, MA
- MP 056 **Protein Networks in Synaptic Vesicles Reveal Heterogeneous and Macromolecular Complexes that Mediate Signal Transduction in neuRons;** Sabine Wittig¹; Carla Schmidt¹; ¹HALOmem, University of Halle, Halle / Saale
- MP 057 **Topographical Characterization of COSMC Using Hydroxyl Radical Protein Footprinting by Fast Photochemical Oxidation of Proteins;** Niloofer Abolhasani Khaje¹; Pradeep Kumar Prabhakar²; Kelley W Moremen²; Joshua S. Sharp¹; ¹Department of Biomolecular Sciences, University of Mississippi, University, MS; ²Complex Carbohydrate Research Center, University of Georgia, Athens, GA
- MP 058 **Starfish Relaxin-Type Dimeric Peptide Cross-Linked by Disulphide Bridges analysed by High Collision Energy (HCD) Fragmentation and Stavrox Software;** Cleidiame Zampronio¹; Ming Lin²; Masatoshi Mita³; Michaela Egertová²; Alexandra M Jones¹; Maurice R Elphick²; ¹University of Warwick, Coventry, UK; ²Queen Mary University of London, London, UK; ³Tokyo Gakugei University, Tokyo, Japan
- MP 059 **Revealing Tertiary Structural Interactions of the Cellular Prion Protein through Chemical Cross-linking and Mass Spectrometry;** Deborah R. Leon¹; Alex J. McDonald¹; Christian F. Heckendorf¹; Mark E. McComb¹; Philip C. Andrews²; David A. Harris¹; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²University of Michigan, Ann Arbor, MI
- MP 060 **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}; Petr Man^{1,2}; Petr Novak^{1,2}; ¹BIOCEV - Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; ²Faculty of Science, Charles University, Prague, Czech Republic
- MP 061 **Application of MS2-PD-MS3 Workflow for Large-Scale Identification of Cross-Linked Peptides;** Ievgen Motorykin¹; Kumar Yugandhar²; Jin Liang²; Elizabeth T. Anderson¹; Robert W. Sherwood¹; Haiyuan Yu²; Sheng Zhang¹; ¹Mass Spectrometry and Proteomics Facility, Institute of Biotechnology, Cornell University, Ithaca, NY; ²Weill Institute for Cell and Molecular Biology, Department of Biological Statistics and Computational Biology, Cornell University, Ithaca, NY
- MP 062 **Development of a Statistic-Based Potential for Chemical Cross-Linking/Mass Spectrometry Derived Constraints for Protein Tertiary Structure Determination;** Allan Jhonathan Ramos Ferrari¹; Leandro Martínez¹; Fabio Cesar Gozzo¹; ¹University of Campinas, Campinas, SP
- MP 063 **X-Ray Hydroxyl Radical Protein Footprinting of Intact, Functional Mitochondria** ; Awuri Asuru¹; Jen Bohon^{2,3}; Janna Kieslar^{1,3}; Mark R. Chance^{1,2,3}; ¹Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; ²Center for Synchrotron Biosciences, Case Western Reserve University, Cleveland, OH; ³Department of Nutrition, Case Western Reserve University, Cleveland, OH
- MP 064 **Characterizing a Plant Receptor Kinase's Three Dimensional Structure using Bottom Up Mass Spectrometry-Based Protein Footprinting;** Pei Liu¹; Benjamin B. Minkoff¹; Miyoshi Haruta¹; Michael R. Sussman¹; ¹Department of Biochemistry and Biotechnology Center, University of Wisconsin, Madison, WI
- MP 065 **Dimethyl Labeling Coupled with Mass Spectrometry for Topographical Characterization of Primary Amines on Monoclonal Antibodies;** Sin-Yi Jhan¹; Li-Juan Huang¹; Shu-Hui Chen¹; ¹National Cheng Kung University, Tainan, Taiwan
- MP 066 **Application of MS3 Experiments to Confidently Identify Cross-linked Peptides;** Bingqing Zhao¹; James P. Reilly²; ¹IU, Bloomington, Indiana; ²Indiana University, Bloomington, IN
- MP 067 **Interpretation of Anomalous Long Crosslinks in Ribosome Crosslinking;** Santosh A Misal¹; James P. Reilly²; ¹Indiana University Bloomington, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- MP 068 **Defining the Structural Dynamics of Cullin-RING Ligase Complexes Using a Novel Multiplexed Quantitative Cross-linking Mass Spectrometry Strategy;** Clinton Yu¹; Haibin Mao²; Alexander Huszaugh¹; Rosa Viner³; Eric Novitsky¹; Scott Rychnovsky⁴; Lan Huang⁴; ¹University of California, Irvine, Irvine, CA; ²University of Washington, Seattle, WA; ³ThermoFisher, San Jose, CA; ⁴University of California, Irvine, Irvine, CA
- MP 069 **Crosslinking Mass Spectrometry (XL-MS) Probes Changes in Protein Domain Structures and Distinguishes Rigid from Flexible Domains;** Lolita Piersimoni¹; Manolo D Plasencia¹; Hollis D Showalter²; Philip C Andrews^{1,3,4}; ¹Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; ²Department of Medicinal Chemistry, 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
- MP 070 **Sequencing the RNA Moiety of Peptide-Oligonucleotide Cross-Links by nanoLC-ESI-MS/MS;** Aleksandar Chernev^{1,2}; Kuan-Ting Pan¹; Uwe Pleßmann¹; Henning Urlaub^{1,2}; ¹Max Planck Institute for Biophysical Chemistry, Goettingen; ²University Medical Center, Goettingen, Germany
- MP 071 **A Software Pipeline for Identifying and Validating Chemical Crosslink Sites in Nonspecifically-Digested LC-MS/MS Samples;** Mark E. Adamo¹; Scott A. Gerber¹; Andrew V. Grassetti¹; ¹Dartmouth College, Lebanon, NH

CARBOHYDRATES I 072 - 098

- MP 072 **Uromodulin Isolation and Its Glycosylation Analysis by nanoLC-MS/MS;** Haiying Li¹; Stephen Kostel¹; John Froehlich¹; Richard S. Lee¹; ¹Boston Children's Hospital, Boston, MA
- MP 073 **Automated Characterization of Isomeric N-glycans using Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS);** Rui Zhang¹; Xue Dong²; Yehia Mechref²; Haixu Tang¹; ¹Indiana University Bloomington, Bloomington, IN; ²Texas Tech University, Lubbock, TX
- MP 074 **Development of a Multi-Dimensional HPLC-MS Method For Heparin/Heparan Sulfate Oligosaccharide Analysis;** Hao Liu¹; Morgan Stickney²; Jonathan I Amster²; Joshua S. Sharp¹; ¹Department of BioMolecular Sciences, The University of Mississippi, Oxford, MS; ²Department of Chemistry, University of Georgia, Athens, GA
- MP 075 **N-glycosylation Analysis of mAbs by CESI-MS at the Glycopeptide and Released Glycan Levels;** Jenny Albanese¹; Marton Sziget²; Bryan Fonslow³; Andras Guttman³; Edna Betgovarguez³; ¹SCIEX, Redwood City, CA; ²University of Debrecen, Debrecen, Hungary; ³Sciex, Brea, CA



- MP 076 **Skyline™-based Quantitative N-glycomics Reveals Altered Expression of Paucimannosidic N-glycans of Mouse Brain Tissues upon Neuropathic Pain Induction;** Christopher Ashwood^{1,2}; Vicky Staikopoulos³; Arun V Everest-Dass^{1,2}; Morten Thaysen-Andersen²; Mark R Hutchinson^{3,4}; Nicolle H Packer^{1,2}; ¹ARC Centre of Excellence in Nanoscale Biophotonics, Macquarie University, Sydney, Australia; ²Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, Australia; ³ARC Centre of Excellence in Nanoscale Biophotonics, The University of Adelaide, Adelaide, Australia; ⁴School of Medicine, The University of Adelaide, Australia
- MP 077 **Mild Acid Dissociation toward Defined Oligosaccharide Groups (MADDOG): A Universal Method for Structural Characterization of Polysaccharides by Nano-HPLC-Chip/Q-TOF Mass Spectrometry;** Matthew J. Amicucci¹; Ace G. Galermo²; Guy Treves²; Carlito B. Lebrilla²; ¹UC Davis Agricultural and Environmental Chemistry Graduate Group, Davis, CA; ²UC Davis Department of Chemistry, Davis, CA
- MP 078 **Sequence Analysis of Proteoglycan Decorin and Other Large Chain Glycosaminoglycan MS2 Using Automated Analysis Software;** Jiana Duan¹; Agyekum Isaac¹; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA
- MP 079 **A Method for Distinguishing Arm-Specific Sialylation of Unsaturated Multiple-Antennae N-linked Glycan Isomers using Exoglycosidase Digestion by HT-PGC LC-MS/MS;** Chein-Hung Chen¹; Ya-Ping Lin¹; Fang-Chi Iliu¹; Chi-Lin Wu¹; Jung-Lee Lin¹; Chung-Hsuan Chen¹; ¹Academia Sinica, Taipei, Taiwan
- MP 080 **Comparison of InstantPC and Traditional N-Glycan Labeling Dyes;** John Yan¹; Andres Guerrero¹; Steven Mast¹; Emily Dale¹; Ted Haxo¹; Aled Jones¹; ¹ProZyme, Hayward, CA
- MP 081 **Automated and Rapid Characterization of Low-Molecular-Weight Heparin Oligosaccharides Using TripleTOF 5600 Mass Spectrometer with SimGlycan Software;** Ningombam Sanjib Meitei^{1,2}; Rajesh Pujari¹; Arun Apte²; Annu Uppal³; ¹PREMIER Biosoft, Indore, India; ²PREMIER Biosoft, Palo Alto, CA; ³SCIEX, Gurgaon, India
- MP 082 **High Throughput Analysis of N-Glycans Released from Biosimilar Glycoproteins;** Zoltan Szabo¹; Shanhua Lin¹; Dietmar Reusch²; Aled Jones³; John Yan³; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Roche Diagnostics GmbH, Penzberg, Germany; ³ProZyme, Hayward, CA
- MP 083 **LC-MS/MS Isomeric Profiling of Permethylated N-Glycans Derived from Serum Haptoglobulin of Hepatocellular Carcinoma (HCC) and Cirrhotic Patients;** Yifan Huang¹; Shiyue Zhou¹; Jianhui Zhu²; David M. Lubman²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²University of Michigan, Ann Arbor, MI
- MP 084 **Isomeric Complexity of Glycosylation in MCF-7 and MDA-MB-231 Cell Lines Revealed by Detailed Analysis with Ion Trap Mass Spectrometry;** David Ashline^{1,2}; Hailong Zhang²; Vernon N. Reinhold²; ¹Glycan Connections, Dover, NH; ²University of New Hampshire, Durham, NH
- MP 085 **16-plex/32-plex LC-MS Analysis of Isotopically Permethylated N-glycans Derived from Biological Samples;** Xue Dong¹; Wenjing Peng¹; Yifan Huang¹; Seth D Williamson¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- MP 086 **Microscale Chemical Release of O-linked Oligosaccharides by RAIDR;** Lucas Veillon¹; Ahmed Hussein^{1,2}; Byeong G Cho¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²Alexandria University, Alexandria, Egypt
- MP 087 **Structure Analysis of Glycosaminoglycan Intermediate Oligosaccharides Elongated on β-xylosides;** Yuuya Otsuka^{1,2}; Toshinori Sato²; ¹Seikagaku Corporation, Higashiyamato-shi, Japan; ²Department of Biosciences and Informatics, Keio University, Yokohama, Japan
- MP 088 **Effectiveness of N-linked Glycan Release: A Quantitative Comparison of Chemical Release versus PNGase F Release Protocols;** David Fischler¹; Ron Orlando¹; ¹Complex Carbohydrate Research Center, University of Georgia, Athens, GA
- MP 089 **Mass Spectrometry-Based Quantitative Analysis for Decoding Site-Specific Alteration of Sialoglycoproteome in EGFR-subtypes of Non-Small Cell Lung Cancers;** Yi-Ju Chen¹; Yu-Hsien Lin²; Ta-Chi Yen¹; Kay-Hooi Khoo³; Yu-Ju Chen¹; ¹Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; ²Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; ³Institute of Biological Chemistry, Taipei City, Taiwan
- MP 090 **Purification of Permethylated N-glycans by using Carbon Nanoparticles: Enhancing Sensitivity and Mass Accuracy;** Jieqiang Zhong¹; Alireza Banazadeh¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- MP 091 **A Universal Approach to linkage-Specific Derivatization for Sialic Acids on Glycopeptides;** Takashi Nishikaze¹; Sadanori Sekiya¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan
- MP 092 **Exploring the Species-specific Glyco-biosynthesis via Nano-LC/MS and LC/MS/MS for the Development of Humanized Mouse Model;** Dan Bi Park^{1,2,3}; Sumin Kim^{2,3}; Jeong Gu Kang⁴; Yong-Sam Kim⁴; Jong Shin Yoo⁵; Jeong-Heon Ko⁴; Hyun Joo An^{1,2}; ¹Asia Glycomics Reference Site, Chungnam National University, South Korea; ²Graduate School of Analytical Science and Technology, Daejeon, South Korea; ³Asia Glycomics Reference Site, Daejeon, South Korea; ⁴Korea Institute of Bioscience and Biotechnology, Daejeon, South Korea; ⁵Korea Basic Science Institute, Cheongju, Chungbuk
- MP 093 **Isomeric Separation and identification of Standard Glycans and Glycans in Model Glycoproteins by PGC-LC-MS/MS at High Temperature;** Aiyang Yu¹; Yifan Huang²; Shiyue Zhou²; Xue Dong²; Yehia Mechref²; ¹Texas Tech University, Lubbock, TX; ²Texas Tech University, Lubbock, TX
- MP 094 **Carbon Nanoparticles and Graphene Nanosheets as MALDI Matrices in Glycomics: A New Approach to Improve Glycan Profiling in Biological Samples;** Alireza Banazadeh¹; Wenjing Peng¹; Lucas Veillon¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
- MP 095 **Fixed Ligand Kinetic Method to Determine the Preservation of Stoichiometry in the Solvolysis of Carbohydrates;** Zachary Wooke¹; Nicola L. B. Pohl¹; ¹Indiana University, Bloomington, IN
- MP 096 **Detailed Structural Analyses of O-glycan Alditols by High Performance Anion Exchange Chromatography (HPAE) Coupled to Mass Spectrometry;** Zoltan Szabo¹; Niclas G Karlsson²; Dietmar Reusch³; Jim Thayer⁴; Yury Agroskin⁴; Rosa Viner⁵; Gina Tan⁵; Andreas F. Huhmer⁶; Christopher Pohl⁴; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²University of Gothenburg, Gothenburg, Sweden; ³Roche Diagnostics GmbH, Penzberg; ⁴Thermo Fisher Scientific, Sunnyvale, CA; ⁵Thermo Fisher Scientific, San Jose, CA
- MP 097 **The Outermost Surface N-glycomics Analysis of Breast Cancer Cell Lines using PNGase F Digestion on living Cells;** Wenjing Peng¹; Akhila Reddy¹; Jingfu Zhao¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- MP 098 **Isomeric N-glycan Analysis of Breast Cancer Cell Lines using Porous Graphitic Carbon (PGC) Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Mona Goli¹; Wenjing Peng¹; Xue Dong¹; Shiyue Zhou¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX

CLINICAL ANALYSIS I
099 - 119

- MP 099 **Quantitation of Putative Colorectal Cancer Biomarker Candidates in Serum Extracellular Vesicles by Targeted Proteomics**; Takeshi Tomonaga¹; Takashi Shiromizu¹; Jun Adachi¹; ¹Laboratory of Proteome Research, National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan
- MP 100 **Modern Orbitrap Based Mass Spectrometers Detect an Unexpected Multitude of Proteoforms in (Human) Secretory Fluids: PROTEOFORMICS of the Human Tear**; Peter D. Verhaert¹; Peter P. Raus²; Martijn W. Pinkse¹; PAUL THOMAS³; Neil L. Kelleher³; ¹Delft University of Technology, DELFT, Europe; ²Miró Center, Geel, Belgium; ³Northwestern University, Evanston, IL
- MP 101 **iKnife Rapid Evaporative Ionisation Mass Spectrometry (REIMS) Technology in Head and Neck Surgery. A ex vivo Feasibility Study**; Jagtar Dhandra¹; Andrew Schache²; Max Robinson³; Zsolt Bodai⁴; Emma L. White⁴; Burak Temelkuran⁴; Yang Guang-Zhong⁴; Zoltan Takats⁴; ¹Queen Victoria Hospital, East Grinstead, UK; ²University of Liverpool, Liverpool, Merseyside; ³University of Newcastle, Newcastle upon Tyne, UK; ⁴Imperial College London, London, UK
- MP 102 **Investigating Paper Properties for Ion Suppression and Recovery in Paper Spray Mass Spectrometry**; Brandon Bills¹; Jeffrey Kinkade¹; Nicholas Manicke¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- MP 103 **Quantitative Proteomic Analysis of MGMT May Predict Response of Colorectal Cancer Patients to Treatment with Temozolomide**; Yuan Tian¹; Sarit Schwartz¹; Wei-li Liao¹; Fabiola Cecchi¹; Filippo Pietrantonio²; Todd Hembrough¹; ¹Nantomics, Rockville, MD; ²Fondazione IRCCS Istituto Nazionale dei Tumori, Milan, Italy
- MP 104 **Breath Analysis with Thermal Desorption-Field Asymmetric Ion Mobility Spectrometry-Mass Spectrometry: A Rapid and Non-Invasive Means of Screening for Pulmonary-Related Diseases**; Alasdair Edge¹; Lauren Brown¹; Kayleigh Arthur¹; Robert Smith¹; ¹Owlstone Medical Ltd., Cambridge, UK
- MP 105 **Background Proteins in hCG Formulations of Different Manufacturers**; Goran Mitulovic¹; Tanja Panić-Janković¹; ¹Medical University of Vienna, KIMCL, Vienna, Austria
- MP 106 **Requirements for Successful Development of MS-based Protein Assays that Target Unmet Clinical Needs**; Yuri E. M. van der Burgt¹; L. Renee Ruhaak¹; Nico P. M. Smit¹; Fred P. H. T. M. Romijn¹; Arnoud van der Laarse¹; Wilma E. Mesker¹; Rob A. E. M. Tollenaar¹; Magnus Palmblad¹; Manfred Wuhrer¹; Christa M. Cobbaert¹; ¹Leiden University Medical Center, Leiden, Netherlands
- MP 107 **Role of RNase L in Kidney**; Norah Alghamdi¹; Danting Liu¹; Ruhan Wei¹; Aimin Zhou¹; ¹Cleveland State University, Department of Chemistry, Cleveland, OH
- MP 108 **LC-MS-MS Quantitative Analysis of Retinoids and Metabolites in Serum for Research Use**; Rory M Doyle¹; Joshua Kilne¹; ¹Thermo Fisher Scientific, Somerset, NJ
- MP 109 **A New Tool for the Automated Sample Preparation of Whole Blood Samples by LC-MS using a Commercial Autosampler**; Guenter Boehm¹; Christian Berchtold²; Reto Bolliger¹; Renzo Piconi¹; Thomas Preiswerk¹; Goetz Schlotterbeck²; ¹CTC Analytics AG, Zwingen, BL; ²Fachhochschule Nordwestschweiz, Muttenz, Switzerland
- MP 110 **Routine 50uL Serum/Plasma Analysis of Hepcidin-25, Hepcidin-20, Hepcidin-22 and Hepcidin-24 using LC/MS/MS: Diurnal Study**; Benjamin Hunter¹; Robert Trengove¹; Joel Gummer¹; ¹Murdoch University, Murdoch, WA
- MP 111 **Clinical Applications by Direct Coupling of Bio-Compatible SPME Devices to MS via Open-Port Probe Sampling Interface**; Marcos Tascon¹; German Gomez-Rios¹; Chang Liu²; Anna Roszkowska¹; Nikita Looby¹; Nathaly Reyes Garces¹; Don W Arnold²; Tom Covey³; Barbara Bojko^{1,4}; Janusz Pawliszyn¹; ¹Department of Chemistry, University of Waterloo, Waterloo, Ontario; ²SCIEX, Concord, ON, Canada, Canada; ³SCIEX, Redwood City, CA; ⁴Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Nicolaus Copernicus University in Torun, Bydgoszcz, Poland
- MP 112 **Non-invasive HRMS Based Approach for Monitoring of Neonates under Intensive Care**; Alexey S. Kononikhin^{1,2}; Natalia Starodubtseva²; Anna Bugrova²; Maria I. Indeykina³; Vitaliy V Chagovets²; Igor Popov¹; Vladimir Frankevich²; Gennady Sukhikh²; Eugene (Evgeny) Nikolaev^{1,4,5}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²V. I. Kulakov Research Center for Obstetrics, Gynecology and Perinatology, Ministry of Healthcare of the Russian Federation, Moscow, Russia; ³Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; ⁴Skolkovo institute of science and technology, Moscow Region, Russia; ⁵Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia
- MP 113 **Biocompatible Handheld Mass Spectrometry Probe for Nondestructive Tissue Analysis and in vivo Cancer Diagnosis**; Jialing Zhang¹; John Rector¹; John Lin¹; Jonathan H Young¹; Nitesh Katta²; Noah Giese¹; Marta Sans¹; Clara Feider¹; Benjamin C. Ludolph¹; Alena Bensussan¹; Rachel J. DeHoog¹; Kyana Y. Garza¹; Thomas Milner²; Livia S. Eberlin¹; ¹Department of Chemistry, The University of Texas at Austin, Austin, TX; ²Department of Biomedical Engineering, The University of Texas at Austin, Austin, TX
- MP 114 **Comparative Analysis of mRNA Degradation and Protein Degradation in 68 Pairs of Adjacent Prostate Tumor Tissue Samples**; Wenguang Shao¹; Tiannan Guo¹; Nora C Toussaint¹; Ulrich Wagner²; Li Li³; Konstantina Champi³; Yi Zhu¹; Andreas Beyer³; Gunnar Ratsch¹; Peter Wild²; Ruedi Aebersold¹; ¹ETH Zurich, Zurich; ²University Hospital Zurich, Zurich, Switzerland; ³University of Cologne, Cologne, Germany
- MP 115 **Does Supercritical Fluid Chromatography Based Mass Spectrometry Help to Find Biomarker/s for Migraine?**; Kumari Ubhayasekera¹; Rik Bongaards¹; Neil De Kock¹; Jonas Bergquist¹; ¹Uppsala University, Uppsala, Sweden
- MP 116 **Use of Automation to Achieve High Performance SPE**; Mark J. Hayward¹; Jonathan Ho²; Matthew T Hardison³; Martin Johnson³; Thomas Moran²; Kim Gamble⁴; ¹ITSP Solutions and Active Ingredient Technologies, Stockton, NJ; ²Shimadzu Scientific Instruments, Somerset, NJ; ³Assurance Scientific Laboratories, Vestavia, AL; ⁴ITSP Solutions, Hartwell, GA
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- MP 118 **The 3D-REIMS Tissue Atlas – in vivo / ex vivo Validation of Classification Model for Intraoperative Tumor Diagnostics**; Keely Pierzchalski¹; Ludwig Dubois²; Natasja G. Lieuwes²; Marius Hennecken²; Pierre-Maxence Vaysse¹; Ulf P. Neumann³; Steven W.M. Olde Damink⁴; Thorsten Cramer³; Ron M.A. Heeren¹; Tiffany Porta¹; ¹M4i Institute, Division of Imaging Mass Spectrometry, Maastricht University, Maastricht, Netherlands; ²Dept. of Radiation Oncology (Maastro Lab), GROW - School for Oncology and Developmental Biology, Maastricht University Medical Centre, Maastricht, Netherlands; ³RWTH Aachen, Aachen,



- Germany; ⁴Dept. of Surgery, Maastricht University Medical Centre, Maastricht, Netherlands
- MP 119 **Online SFE-SFC-MS for Direct Extraction and Analysis of Designer Drugs in Urine Samples;** Alison Paige Wicker¹; Volodymyr Pauk²; Changling Qiu¹; Karel Lemr²; Vladimir Havlicek²; Kevin A. Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²Palacky University in Olomouc, Olomouc, Czech Republic

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- MP 121 **Development and Application of Magnetic Microbead Affinity Selection Screening (MagMASS) for Novel Retinoid X Receptor- α (RXR α) Anti-Inflammatory Agents;** Ruth Muchiri¹; Rush Michael¹; Elisabeth Walker¹; Richard van Breemen¹; ¹University of Illinois at Chicago, Chicago, IL
- MP 122 **Protein Array-ALIS: A Combined Affinity Selection – Mass Spectrometry / Phenotypic Screening Approach for Identification of Protein Drug Targets;** Elliott Nickbarg¹; Peter J. Dandliker¹; Shuli Yang¹; Nicholas Murgolo²; Scott Walker²; PAUL Mann²; Donna Carr²; Terry Roemer²; Todd Black²; Bruce Beutel¹; ¹Merck & Co., Inc., Boston, MA; ²Merck & Co., Inc, Kenilworth, NJ
- MP 123 **Investigation of the Metabolites of CCK-4 in Human/ Rat Plasma by Ultra-High Performance Liquid Chromatography-Orbitrap Fusion Tribrid Mass Spectrometer;** Li Kong¹; Frederic J Berg¹; ¹ECBC, US Army, Gunpowder, MD
- MP 124 **Physicochemical Properties of Carfentanil, an Ultra-Potent Opioid of Abuse;** Richard J Lawrence¹; Michael G Feasel¹; ¹Edgewood Chemical Biological Center (ECBC), Aberdeen Proving Ground, MD
- MP 125 **Reverse Affinity Screening Technology Enabled by High-Throughput Mass Spectrometry in Drug Discovery;** Ting Song¹; Mark Southern²; John D. McCarter²; ¹Amgen, Thousand Oaks, CA; ²Amgen, Thousand Oaks, CA
- MP 126 **Improvements of the DMPK Workflow Utilizing a Supercritical Extraction – SFC – MS/MS Combination. Systematic Evaluation of the Make-Up Composition;** Andreas Fredenhagen¹; Arnold Demailly¹; Markus Walles¹; Laura Akbal^{1,2}; Caroline Radoch¹; ¹Novartis, Basel; ²Universite de Geneve, Geneva, Switzerland
- MP 127 **WebMetabase: High Resolution Mass Spectrometry Tool to Investigate Peptide Metabolism and Investigate Peptides Cleavage Site Based on Frequency;** Tatiana Radchenko^{1,2}; Christopher Kochansky³; Alison Bateman³; Fabien Fontaine²; Luca Moretoni¹; Ismael Zamora^{1,2}; ¹Universitat Pompeu Fabra, Barcelona, Spain; ²Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; ³Merck & Co., West Point, PA; ⁴Molecular Discovery, London, UK
- MP 128 **Simultaneous Determination of Doxorubicin and Modified Hyaluronan in Mouse Plasma and Its Tissues;** Matej Simek¹; Martina Hermannova¹; Daniela Smejkalova¹; Karel Soucek²; Vladimir Velebny¹; ¹Contipro a.s., Dolni Dobrouc, Czech Republic; ²Academy of Science of the Czech Republic, Brno, Czech Republic
- MP 129 **Metabolite Profiling in Tissues from Whole Body Slices via Improved Liquid Microjunction Surface Sampling followed by LC-HRMS;** Weiqi Chen¹; Lifei Wang¹; Anthony Barros¹; Jinping Gan¹; ¹BMS, Princeton, NJ
- MP 130 **AIMS (Automated in vivo MS System) - A Novel Drug Discovery Software to Boost In Vivo LC-MS/MS Analytics ;** Andreas H. Luippold¹; Wolfgang Rist¹;

- Tom Bretschneider¹; Wolfgang Joerg¹; Christian Spaeth¹; Juergen Weber¹; Siegfried Wild¹; Daniel Bischoff¹; ¹Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Baden Württemberg
- MP 131 **Speedy Characterization of Cyclic Peptide Metabolites in Complex Biological Matrix with integrated LC/MS/MS and MassMetaSite/WebMetaB;** Silvi Chacko¹; Nirmala Ragahavan²; Yue-Zhong Shu²; William Humphreys²; ¹Bristol-Myers Squibb, Pennington, NJ; ²Bristol-Myers Squibb, Princeton, NJ
- MP 132 **Biotherapeutic Analysis using Automated Affinity Purification and Sensitive Intact Protein Based LC/Q-TOF Analysis;** Jing Chen¹; Alex Zhu²; Steve Murphy³; ¹Agilent, Madison, WI; ²Agilent Technologies, Inc., Wilmington, DE; ³Agilent Technologies, Inc., Madison, WI
- MP 133 **Efficient Theranostic System for Hypoxia Mediated Drug Delivery: Rhodamine-Derived Azobenzene Mustards;** Jiyeong Lee¹; Peter Verwilt²; Jiyoun Han³; Sora Mun⁴; AeEun Seok⁴; Arum Park⁴; Jong Seung Kim²; Hee-Gyoo Kang^{1,4}; ¹Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam, South Korea; ²Department of Chemistry, Korea University, Seoul, South Korea; ³Department of Biotechnology, Laboratory of Stem Cells and Tissue Regeneration, College of Life Sciences & Bio Technology, Korea University, Seoul, South Korea; ⁴Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam, South Korea
- MP 134 **Beyond HPLC-MS: Profiling of High Molecular Weight Impurities during Drug Synthesis;** Holger Bauer¹; Hans Griesinger¹; Katerina Matheis¹; Annette Michalski¹; ¹Merck KGaA, Darmstadt, Germany
- MP 135 **Evaluation of a Cyclic Mobility-Enabled Research Platform with Multiple-Pass Ion Geometry for Metabolite Characterisation Studies;** Richard Clayton¹; Catherine Holdsworth¹; Nick Tomczyk²; Kevin Giles²; Jakub Ujma²; Daniel Weston²; ¹Covance, Harrogate, UK; ²Waters Corporation, Wilmslow, UK
- MP 136 **Comprehensive Identification of Drug Targets and Target Engagement Biomarkers by Proteome-Wide CETSA and Chemical Proteomics;** Gabriele Stoehr¹; Melanie Maschberger¹; Johannes Krumm²; Sandra Silingas¹; Thomas Wieland¹; Bernhard Kuster²; Hannes Hahne³; ¹OmicScouts GmbH, Freising; ²Technical University of Munich, Freising, Germany; ³OmicScouts GmbH, Freising, Germany
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- MP 138 **Pharmacokinetic and Metabolomic Profiling of Inhaled Simvastatin in Rhesus Macaque;** Mona Elbadawi-Sidhu¹; Sean Ott²; Jules Larke³; Osamede Enobakhare¹; Jessica Kwok³; Louise Olsen⁴; Amir Zeki²; Oliver Fiehn³; ¹NIH West Coast Metabolomics Center, University of California Davis, Davis, CA; ²Dept. of Internal Medicine, Division of Pulmonary, Critical Care and Sleep Medicine, University of California – Davis, Davis, CA; ³NIH West Coast Metabolomics Center, University of California – Davis, Davis, CA; ⁴California National Primate Research Center, University of California – Davis, Davis, CA
- MP 139 **Metabolite Identification of Fentanyl and Fentanyl Analogs Incubated in Human Hepatocytes;** Ron G. Aoyama¹; Tim J. Stratton²; ¹Gilead Sciences, Foster City, CA; ²ThermoFisher, San Jose, CA
- MP 140 **Systematic Characterizations of Target Kinases and Kinome Reprogramming of Clinically Used Kinase Inhibitors;** Weili Miao¹; Lei Guo¹; Yongsheng Xiao¹; Yinsheng Wang¹; ¹University of California, Riverside, CA



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- MP 142 **Novel Chemoproteomic Approaches for Proteome-wide Characterization of Covalent Drug Binding**; Jarrold Marto; Dana Farber Cancer Instit, Boston, MA
- MP 143 **Broad-Spectrum Kinase Profiling in Live Cells with Lysine-Targeted Sulfonyl Fluoride Probes**; Qian Zhao; Hong Kong Baptist University, Kowloon Tong, Kowloon, China
- MP 144 **Development of a Magnetic Microbead Affinity Selection Screening (MagMASS) UHPLC-MS Assay for the Progesterone Receptor**; Daniel Nosal¹; Michael D Rush¹; Tristesse Burton¹; Richard van Breemen¹; ¹University of Illinois at Chicago College of Pharmacy, Chicago, IL
- MP 145 **Optimization of High-Resolution MS Parameters for an Automated High-throughput Metabolic Stability Assay with Simultaneous Accumulation of Quantitative/Qualitative Data**; David Heim¹; Richard Burton¹; Shelby Anderson¹; Dongting Liu¹; Xiaochun Zhu¹; Heasook Kim-Kang¹; ¹Q2 Solutions, Indianapolis, IN
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- MP 147 **An Open Port Sampling Interface for High-Throughput SPME-MS/MS analysis of *in vitro* ADME Samples**; John Janiszewski¹; Brendon Kapinos²; Sara Smith³; Craig Aurand³; Chang Liu⁴; Tom Covey⁴; German Augusto Gomez-Rios⁵; ¹Pfizer Inc., Groton, CT; ²Pfizer Inc., Groton, CT; ³MilliporeSigma, Bellefonte, PA; ⁴SCIEX, Concord, ON, Canada; ⁵University of Waterloo, Waterloo, Ontario
- MP 148 **Metabolomics and Biochemical Investigation of Anti-adipogenic Diarylheptanoids in *Dioscorea zingiberensis*** C.H. Wright; Dan Du^{1,2}; Haiwei Gu¹; Danijel Djukovic¹; Lisa Bettcher¹; Daniel Raftery¹; Meng Gong^{1,2}; ¹University of Washington, Seattle, WA; ²West China-Washington Mitochondria and Metabolism Center, West China Hospital, Sichuan University, Chengdu, China
- MP 149 **Optimum Use of Large Volume Injection Techniques for Metabolite Profiling Studies – Low Radioactivity or Low Dose Exploratory Samples**; Jessica Shoultz¹; Shelby Anderson²; David Heim¹; ¹Q2 Solutions, Indianapolis, IN; ²Q2 Solutions, Carmel, IN
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- MP 154 **Certifying a New Ambient-Level Cr(VI) Reference Standard in Soil Matrix and Determining Cr(VI) in NIST 3280 Dietary Supplement Reference Standard**; James Henderson¹; Patrick Benecewicz¹; Weier Hao¹; Logan Miller¹; Matt Pamuku²; Jennifer Crawford²; Teresa Switzer³; Vasile Furdul³; Pamela Wee⁴; Stuart Procter⁵; Francine Walker⁶; Bob O'Brien⁷; H. M. Skip Kingston¹; ¹Duquesne University, Pittsburgh, PA; ²Applied Isotope Technologies Company, Pittsburgh, PA; ³Ministry of Environment, Toronto, ON, Canada; ⁴Agilent Technologies Inc., Santa Clara, CA; ⁵Metrohm USA, Inc., Riverview, FL; ⁶Chemical Solutions Company, Harrisburg, PA; ⁷Sigma Aldrich Company, St. Louis, MO
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- MP 159 **Investigating the Fragmentation Chemistry of Isomeric Polycyclic Aromatic Hydrocarbon Derivatives**; Maha T. Abutokaikah¹; Curtis M. Stump¹; Eli S. LaChance¹; Christopher D. Spilling¹; Benjamin B. Bythell¹; ¹University of Missouri–St. Louis, St. Louis, MO
- MP 160 **High Performance Thin Layer Chromatography with Atmospheric Solids Analysis Probe Mass Spectrometry for analysis of gasoline additives**; Mathieu Beaumesnil^{1,2}; Anna Luiza Mendes Siqueira^{1,2}; Marie Hubert-Roux²; Amandine Racaud¹; Carlos Afonso²; Yang Bai¹; ¹TOTAL Marketing & Services, Research Center, 69360 Solaize, France; ²Normandie Univ., UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France
- MP 161 **Direct Analysis of a Butane Combustion Flame by using a High Resolution Multi-Turn Mass Spectrometer**; Koji Okuda¹; Andrew John Dane¹; Takashi Satoh²; Yukinori Yahata²; Robert B Cody¹; ¹JEOL USA Inc., Peabody, MA; ²JEOL Ltd., Akishima, Japan
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- MP 163 **Molecular characterization of Heavy Petroleum Products using Data Processing-Enhanced 7 T LTQ FT-ICR MS**; Florian Albricux¹; Lyes Assam¹; Konstantin O. Nagornov²; Anton N. Kozhinov²; Yury O. Tsybin²; ¹IFPEN, Solaize, France; ²Spectroswiss Sàrl, Lausanne, Switzerland
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- MP 165 **Characterization of organic compounds in Process Water from Colombian Oil Wells**; Diana Catalina Palacio Lozano^{1,2}; Enrique Mejía-Ospino¹; Mark P Barrow²; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²University of Warwick, Coventry, Midlands
- MP 166 **Molecular Characterization of Naphthenic Acids Extracted from a Heavy Crude Oil using MALDI FTICR Mass Spectrometry**; Jefferson A. Valencia-Dávila¹; Matthias Witt²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 167 **Selective Ionization of Vanadyl Porphyrins Extracted from South American heavy oils using a Novel Electron Transfer MALDI Matrix**; Deisy Giraldo-Dávila¹; Martha L. Chacón-Patiño¹; Juan S. Ramírez-Pradilla¹; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia
- MP 168 **Application of On-line Liquid Chromatography Coupled to Ultra-High Resolution 21 T FT-ICR Mass Spectrometry for Petroleum Analysis**; Donald F. Smith¹; Steven M. Rowland^{1,2}; Greg T. Blakney¹; Yuri E. Corilo^{1,2}; Christopher L. Hendrickson^{1,2,3}; Ryan P. Rodgers^{1,2,3}; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ²Future Fuels Institute, Florida State University, Tallahassee, FL; ³Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- MP 169 **Estimation of Confidence in Assigning True Molecular Formulae of Complex Mixtures**; Yuri E. Corilo^{1,2}; Melaine C. De Oliveira³; Donald F. Smith¹; Ryan P. Rodgers^{2,4,5}; Christopher L. Hendrickson^{2,4,5}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Florida State University, Tallahassee, Florida; ³Department of Statistics, Florida State University, Tallahassee, FL; ⁴National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ⁵Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- MP 170 **Direct-coupling of Different Chromatographic Separation Methods to Ultrahigh Resolution Mass Spectrometry for the analysis of crude oil and its Fractions**; Wolfgang Schrader¹; Alessandro Vetere²; ¹Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr; ²Max-Planck-Institut für Kohlenforschung, Mülheim / Ruhr, Germany
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- MP 173 **Comparison of Atmospheric Pressure Chemical Ionization and Field Ionization Mass Spectrometry for the Analysis of Large Saturated Hydrocarbons**; Yuyang Zhang¹; Chunfen Jin¹; Jyrki Viidanoja²; Jeremy Manheim¹; Mingzhe Li¹; Hilkka Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Neste Corporation, Finland
- MP 174 **Differentiation of Isomeric Hydrocarbon Ions Containing Five- and Six-Membered Naphthene Rings by using Energy-Resolved Medium Energy Collision-Activated Dissociation (MCAD)**; Mark Romanczyk¹; Jyrki Viidanoja²; Hilkka Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Thermo Fisher Scientific, Vantaa, Finland
- MP 175 **Structural Determination of Polycyclic Aromatic Hydrocarbons by Ion Mobility Mass Spectrometry**; Priscila M. Lalli^{1,2}; Yuri E. Corilo^{2,3}; Martha L. Chacón-Patiño³; RYAN P. RODGERS^{2,3,4}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, Florida State University, Tallahassee, FL; ³National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ⁴Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- MP 176 **Direct Infusion APCI MS Analysis of Mixtures of Large Saturated Hydrocarbons by Using Different Hydrocarbon Solvents**; Jeremy Manheim¹; Yuyang Zhang¹; Chunfen Jin¹; Jyrki Viidanoja²; Hilkka Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Neste Corporation, Finland
- MP 177 **Acceleration of Field-Activated TiO₂-catalyzed Oil Degradation in Microdroplets**; Yin-Hung Lai¹; Zhenpeng Zhou¹; Chanbasha Basheer²; Richard N Zare¹; ¹Stanford University, Stanford, CA; ²Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia
- MP 178 **FT-ICR-MS Data Provide Structural Features of Heavy Crude Oil Components**; Cristian Blanco-Combariza¹; Marianny Y Combariza¹; Cristian Blanco-Tirado¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia
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- MP 180 **Prediction of the SARA Analysis of Colombian Crude Oils Using APPI(+)-FTICR MS Coupled to PLS with GA Variable Selection**; Enrique Mejía-Ospino¹; Diana Catalina Palacio¹; Jorge A. Orrego-Ruiz²; Jader E. Guerrero¹; Rafael Cabanzo¹; ¹Universidad Industrial de Santander, Bucaramanga, SDER; ²Instituto Colombiano de Petróleos (ICP), Piedecuesta, Colombia
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- MP 183 **Detection of Harmful Carbonyl Compounds in E-Cigarette Liquids via *in-situ* Derivatization Nano-Electrospray Ionization Mass Spectrometry**; Tavleen K. Kochar¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- MP 184 **Investigation of Extracted and Leached Analytes from Packaging Materials with GC-MS and High Resolution MS**; Elizabeth Humston-Fulmer¹; Joe Binkley¹; ¹LECO Corporation, Saint Joseph, MI
- MP 185 **Direct Analysis of Glyphosate in wine with No Sample Preparation using an LC-MS/MS System with a Stay Clean Source**; Sharanya Reddy¹; Matteo Meglioli²; Frank Kero¹; ¹PerkinElmer, Shelton, CT; ²Mosti Mondiale Inc, Québec, QC, Canada



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- MP 187 **A Multi-Laboratory Comparison of MS Platforms for the Targeted Analysis of Peanut in Food;** Victoria Lee¹; Rebekah L. Sayers¹; Ivona Baricevic-Jones¹; Carol-Ann Costello¹; Sabine Baumgartner²; Christine H. Parker³; Gavin O'Connor⁴; Philip Johnson⁵; E. N. C. Mills¹; ¹University of Manchester, Manchester, UK; ²University of Natural Resources and Life Sciences - BOKU, Vienna, Austria; ³FDA Center for Food Safety, College Park, MD; ⁴JRC IRMM, Geel, Belgium; ⁵University of Nebraska, Lincoln, NE
- MP 188 **Determination of multiple pesticide residue in Green Chilli by GC-MS/MS using Modified QuEChERS as an Extraction Method;** Sanket Chiplunkar¹; Dheeraj Handique¹; Ankush Bhone¹; Prashant Hase¹; Durvesh Sawant¹; Nitish Suryawanshi¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 189 **Highly Sensitive and Rapid Analysis of Synthetic dyes in Sea Food by LC/MS/MS;** Shailesh Damale¹; Anant Lohar¹; Shailendra Rane¹; Purushottam Sutar¹; Ashutosh Shelar¹; Deepti Bhandarkar¹; Rashi Kochhar¹; Jitendra Kelkar¹; Pratap Rasam¹; Ajit Datar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 190 **Determination of Polycyclic Aromatic Hydrocarbons in a Candidate Yerba Mate Standard Reference Material by GC-MS;** Jacolin A. Murray¹; Michele M. Schantz¹; Laura J. Wood¹; Melissa M. Phillips¹; Stephen A. Wise^{1,2}; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²National Institutes of Health, Bethesda, MD
- MP 191 **LC-MS/MS and DART-HRMS Screening of Beverages for Sweeteners;** Luke K Ackerman¹; Nicole Shyong¹; ¹FDA Center for Food Safety, College Park, MD
- MP 192 **A Novel Fast and Simple Quantification Method for Vitamins, Complements and contaminants in Milk Infant Formulas by LC-MS/MS;** Aurore Jaffuel¹; Thierry Legoupil¹; Alban Huteau¹; ¹Shimadzu France, Paris, France
- MP 193 **Improving Gas Chromatograph-Mass Spectrometer System Longevity for Multi-Residue Pesticide Methods in Matrix Through Inert Microfluidic Retention Gap Technology;** Rebecca Veeneman¹; Matthew Giardina¹; ¹Agilent Technologies, Wilmington, Delaware
- MP 194 **Sample Profiler: A Cloud Based Application for Confirming Food Authenticity;** Srividya Kailasam¹; Ralf Tautenhahn²; Tim J. Stratton²; ¹ThermoFisher Scientific, Bangalore, India; ²ThermoFisher, San Jose, CA
- MP 195 **Application of SFC-MS/MS for the Quantification of Highly Polar Pesticides in a Range of Food Samples;** David Baker¹; Chris Titman¹; Jonathan Horner²; Neil Loftus¹; ¹Shimadzu, Manchester, UK; ²Scientific Analysis Laboratories, Cambridge, UK
- MP 196 **Screening of Pesticides and other contaminants in Food Matrices using a Novel High Resolution GC/Q-TOF with Low-Energy Capable EI Source;** Kai Chen¹; Jennifer Sanderson¹; ¹Agilent Technologies, Santa Clara, CA
- MP 197 **Using Pressurized Liquid Extraction for the Extraction and Analysis of Pesticides in Cannabis Samples;** Philip M. Germansderfer¹; Hamid R. Shirkhan¹; ¹Fluid Management Systems, Watertown, MA
- MP 198 **Direct Analysis of glyphosate and Similar Polar Pesticides in Various Food Matrices;** Dimple Shah¹; Euan Ross²; Benjamin Wuyts²; Eimear McCall²; Gareth Cleland¹; Kenneth Rosnack¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- MP 199 **Automated Extraction and Clean Up of POPs Using a Green Low Solvent System;** Hamid R. Shirkhan¹; Waleed Hassan¹; ¹Fluid Management Systems, Watertown, MA
- MP 200 **Multiresidue Pesticide Analysis in Fruit and Vegetable Commodities Using Both UPLC and APGC on a Single Mass Spectrometer Platform;** Kari Organtini¹; Eimear McCall²; Gareth Cleland¹; Kenneth Rosnack¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- MP 201 **Advances in Ion Mobility Mass Spectrometry to Further Characterize Contaminants in Food;** Lauren Mullin¹; Gareth Cleland¹; Andrew Baker³; Mike McCullagh⁴; Sara Stead⁴; Kenneth Rosnack¹; Joe Romano¹; ¹Waters Corporation, Milford, MA; ²Örebro University, Örebro, Sweden; ³Waters Corporation, Pleasanton, CA; ⁴Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- MP 202 **Development of a Comprehensive Multiplex Allergen Detection MRM Method for Standardized Food Testing;** Derek Croote¹; Ido Braslavsky²; Karolina M. Krasinska³; Stephen R. Quake¹; ¹Stanford University, Stanford, CA; ²Hebrew University, Jerusalem, Israel; ³Stanford University Mass spectrometry, Stanford, CA
- MP 203 **Target Peptide Identification for the Mass Spectrometric Detection of Soy Proteins in Food Matrices;** Shimin Chen¹; Charles Yang²; Melanie Downs¹; ¹Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE; ²Thermo Fisher Scientific, San Jose, CA
- MP 204 **Analysis of Polychlorinated Biphenyls in Coffee using Automated Extraction and Reduced Solvent Volume Clean Up;** Thomas G. Hall¹; Alexander Sharapov¹; ¹Fluid Management Systems, Watertown, MA
- MP 205 **Fully Automated Derivatization -Quantification of Glyphosate and AMPA in Beer using a Standard UHPLC-MS/MS System;** Julia Sander¹; Anja Grüning¹; Robert Ludwig¹; Philipp Jochems¹; ¹Shimadzu Europa GmbH, Duisburg, Germany
- MP 206 **Analysis of Mycotoxins in Cereal and Corn without Derivatization via LC-MS/MS with Time-Managed MRMs;** Wilhad Reuter¹; Avinash Dalmia¹; ¹PerkinElmer Inc, Shelton, CT
- MP 207 **A Data-dependent Workflow for Selection of Peptide Targets for Robust Detection of allergens in Difficult Food Matrices;** Justin T. Marsh¹; Charles Yang²; Philip Johnson¹; ¹University of Nebraska, Lincoln, NE; ²Thermo Fisher Scientific, San Jose, CA
- MP 208 **Fast and Extended Analysis of 213 FDA Regulated Pesticides in Organic and Non-organic Grapes by LC-MS/MS using Time-Managed-MRM;** Joshua Ye¹; Feng Qin¹; Shixin Sun¹; Avinash Dalmia²; Wilhad Reuter²; Sergey Rakov²; Jamie Foss³; Frank Kero³; ¹PerkinElmer LAS Canada Inc, Woodbridge, ON, Canada; ²PerkinElmer Inc, Shelton, CT; ³PerkinElmer, Downers Grove, IL
- MP 209 **Analytical Confirmation of Sildenafil Analogues Adulterated in Dietary Supplements;** Nam Sook Kim¹; Ji Hyun Lee¹; Kyu Yeon Kim¹; Han Na Park¹; Hyoung-Joon Park¹; Taeik Hwang¹; Seok Heo¹; Jeong-Hwa Cho¹; Junhyoung Kim¹; Dong Woo Shin¹; Seongsoo Park¹; Sung-Kwan Park¹; Sun Young Baek¹; ¹Ministry of Food and Drug Safety, Cheongju-si, Chungcheongbuk-do
- MP 210 **Released Volatiles Analysis of Flavor Capsules in Cigarette Filter under Simulated Working Conditions by Headspace-GC×GC-MS;** Xiangyu Li¹; Hongfei Zhang¹; Xingyi Jiang¹; Yanbo Luo¹; Fengpeng Zhu¹; Shaocong Hu¹; Yongqiang Pang¹; ¹China National Tobacco Quality Supervision & Test Centre, Zhengzhou, China
- MP 211 **Fast and Robust Multiresidue Analysis of Highly Polar Pesticides by Ion Chromatography Coupled to High Resolution Mass Spectrometry;** Łukasz Rajski¹



- Francisco José Díaz-Galiano¹; Víctor Cutillas¹; Amadeo R. Fernández-Alba¹; ¹European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, Almería, Spain
- MP 212 **Infant Exposure to Arsenic and Lead From Rice Cereal and Bottled Water**; Marc E. Engel¹; Donald M Axelrad²; ¹FDACS, Tallahassee, FL; ²Florida A&M University College of Pharmacy and Pharmaceutical Sciences Institute of Public Health, Tallahassee, FL
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- MP 213 **Multiplexing Hard and soft Electron Ionisation for Improved Speciation of Cannabinoids**; Chris Hall¹; Natasha Spadafora¹; Laura McGregor¹; Matthew Edwards²; Pete Grosshans¹; Nick Bukowski¹; ¹Markes International, Llantrisant, Cardiff; ²SepSolve Analytical, Peterborough, UK
- MP 214 **Screening of Drugs of Abuse and Pesticides in Liver following Homogenization and Supported Liquid Extraction (SLE) prior to GC/MS Analysis**; Rhys Jones¹; Katie-Jo Teehan¹; Lee Williams¹; Geoff Davies¹; Helen Lodder¹; Adam Senior¹; Alan Edgington¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹Biotage GB Limited, Cardiff
- MP 215 **Direct Detection of Security Relevant Substances on Surfaces via Ambient Pressure Laser Desorption Mass Spectrometry**; René Reiss¹; Sven Ehler^{1,2}; Ralf Zimmermann^{1,3}; ¹University of Rostock, Department of Analytical Chemistry, Rostock, Germany; ²Photonion GmbH, Schwerin, Germany; ³Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, München, Germany
- MP 216 **Chemical Imaging of Cyanoacrylate Fumed Fingerprints Using MALDI-Orbitrap**; Kelly O'Neill¹; Paige Hinners¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- MP 217 **Rapid Screening and Determination of New Psychoactive Substances by Direct Analysis in Real Time Mass Spectrometry and LC/QTOFMS**; Honggang Nie¹; Xianjiang Li¹; Zhendong Hua²; Wei Pan¹; Xiaofang Fu¹; ¹Peking University, Beijing, Beijing; ²National Narcotics Laboratory, Beijing, China
- MP 218 **Chemical Identification in Latent Fingerprints for Lifestyle Determination**; Paige Hinners¹; Kelly O'Neill¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- MP 219 **An LC-QTOF-MS Assay for Post-Mortem Drug Screening in Dental Hard Tissue Samples**; Laura M. Huppertz¹; Miriam Klima¹; Miriam C. Kualess²; Markus J. Altenburger²; Volker Auwärter¹; Merja A. Neukamm¹; ¹Institute of Forensic Medicine, Forensic Toxicology, Medical Center - University of Freiburg, Freiburg, Germany; ²Center for Dental Medicine, Department of Operative Dentistry and Periodontology, Medical Center - University of Freiburg, Freiburg, Germany
- MP 220 **Paper Cone Spray Ionization Sources Featuring Integrated Extraction and Filtration for On-Site Forensic Applications**; William L. Fatigante¹; Zachary E. Lawton¹; Alessandra M. Bruno¹; Shahnaz Mukta¹; Michael C. Gizzi¹; Christopher C. Mulligan¹; ¹Illinois State University, Normal, IL
- MP 221 **Development of Laser Ablation Direct Analysis in Real Time Imaging Mass Spectrometry (LADI-MS): Applications to Forensics Imaging**; Kristen Fowble¹; Rabi A Musah¹; ¹University at Albany, Albany, NY
- MP 222 **Speciation of Antimony in Biological Samples by Liquid Chromatography-Inductively Coupled Plasma-Mass Spectrometry**; Yuko Kazui¹; Yasuo Seto¹; Shinichi Suzuki¹; Yasuhiro Suzuki¹; Ritsuko Sugita¹; Hikoto Ohta¹; Masaaki Kasamatsu¹; Hajime Miyaguchi¹; Takao Igawa¹; ¹National Research Institute of Police Science, Kashiwa
- MP 223 **Collection and Analysis of Drugs using Electrospun Nanofibers with Microfluidic Extraction and Tandem Mass Spectrometry**; Yufei Chen¹; Pei Zhu²; Xiangwu Zhang¹; Nelson Vinuesa²; ¹North Carolina State University, Raleigh, NC; ²North Carolina State University, Raleigh, NC
- MP 224 **The Detection of Designer Drugs from Plasma via Paper Spray Mass Spectrometry**; Greta Jakstonyte Ren¹; Nicholas Manicke¹; ¹IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
- MP 225 **Separation and Identification of Organic Compounds in Gun Powders Using LC-MS Techniques**; Danielle Kirby¹; Michael J. Van Stipdonk¹; Stephanie J. Wetzel¹; Logan Miller¹; Kyle Brown¹; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA
- MP 226 **LC-MS/MS Analysis of Hair Samples for the Detection of Prohibited Substances in Equine and Canine Sport**; Bob Gray¹; Marjaana Viljanto¹; Eleanor Menzies¹; Stephanie Thompson¹; Erin Crum^{1,2}; James Scarth¹; ¹LGC Ltd, Middlesex; ²LGC Ltd US, Lexington, KY
- MP 227 **Detection of Antifungal Drugs and Their Main Metabolites in Human Urine by LC-MS-based Techniques: Implications in Doping Analysis**; Monica Mazzarino¹; Fabio Comunità¹; Xavier de la Torre¹; Francesco Botrè^{1,2}; ¹Antidoping Laboratory of Rome, Rome, Italy; ²Università degli studi di Roma "Sapienza", Rome, Italy
- MP 228 **Using Differential Mobility Spectrometry to Separate Chiral Compounds: Amphetamines**; J. Larry Campbell¹; J.C. Yves Leblanc²; Chang Liu²; ¹SCIEX, Concord, ON, Canada; ²SCIEX, Concord, ON, Canada, ON, Canada
- MP 229 **Multivariate Data Interpretation of Direct Biomarkers of Ethanol Consumption for Forensic Purposes**; Marco Vincenti^{1,2}; Eugenio Alladio^{1,2}; Martyna Agnieszka³; Alberto Salomone²; Valentina Pirro⁴; Grzegorz Zadora^{3,5}; ¹Dept. of Chemistry, Università di Torino, Torino, Italy; ²Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Orbassano (Torino), Italy; ³Department of Analytical Chemistry, The University of Silesia, Katowice, Poland; ⁴Dept. of Chemistry, Purdue University, West Lafayette, IN; ⁵Institute of Forensic Research, Krakow, Poland
- MP 230 **Compact Mass Spectrometer (CMS) Analysis of Uniformly ¹³C-labeled Amino Acids to Identify Authentic Therapeutic Drugs and Protect against Counterfeits**; Daniel Eikel¹; Simon J. Prosser²; Chris Beecher³; ¹Advion Inc., Ithaca, NY; ²Advion Inc., Ithaca, NY; ³IROA Technologies, Bolton, MA
- MP 231 **Development of a Portable nLC-EI-MS**; Clyde Hale¹; Mehdi Moini²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
- MP 232 **Comparison between DSA TOF-MS and DART TOF-MS for the Analysis of Writing Inks**; Nicholas L. Drury¹; Mehdi Moini²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
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- MP 234 **Sonic Versus ESI Ionization for Noncovalent Interactions**; Abdil Ozdemir¹; Mustafa Gulen¹; Jung-Lee Lin²; Chung-Hsuan Chen²; ¹Sakarya University, Adapazari, Sakarya; ²Academia Sinica, Taipei, Taiwan
- MP 235 **Opposite Polarity Electrical Charge on Electrospayed Bacterial Spores: Implications for Electrospray Mechanism**; Jiuzhi Gao¹; Ames Ettinger¹; Richard A. Robison¹; Daniel E. Austin¹; ¹Brigham Young University, Provo, UT



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- MP 237 **Comparing the Effects of Additives on Protein Analysis by DESI and ESI;** Elahe Honarvar¹; Andre R. Venter¹; ¹Western Michigan University, Kalamazoo, MI
- MP 238 **Understanding Electrospray Ionization Mechanisms of Biomolecules using In-Plume Laser-Induced Fluorescence;** Prince Tiwari¹; Martin F. Czar¹; Renato Zenobi¹; ¹ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland
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- MP 241 **Electron Transfer Dissociation and Collision-Induced Dissociation of Trivalent Metal-Adducted Oligosaccharides;** Ranelle Schaller-Duke¹; Carolyn J. Cassady²; ¹The University of Alabama, Tuscaloosa, AL; ²The University of Alabama, Tuscaloosa, AL
- MP 242 **Exploring Halide Anion Affinity of Cyclodextrins by Electrospray Ionization Mass Spectrometry and Molecular Modeling;** Chongsheng Xu¹; Yanqiu Chu¹; Chuan-Fan Ding¹; ¹Fudan University, Shanghai, Shanghai
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- MP 244 **Energy Deposition During Electron Ionization of Molecules;** Karl Irikura; Natl Inst Standards & Tech, Gaithersburg, MD
- MP 245 **Theoretical Studies on Reactions of Gas Phase Ions with Water Covered α -quartz Surfaces;** Alexander Haack¹; Walter Wissdorf¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal
- MP 246 **Developing a Fundamental Understanding of Inlet Ionization through Density Functional Theory (DFT);** Wen-Jing Zhang¹; Bishnu Thapa¹; H. Bernhard Schlegel¹; Sarah Trimpin¹; ¹Department of Chemistry, Wayne State University, Detroit, MI
- MP 247 **Theoretical Investigation of the Reactivity of para-Benzynes Ions Toward Cyclohexane in the Gas Phase;** Jacob R. Milton¹; Huaming Sheng²; Xin Ma¹; John J. Nash¹; Hilkka I. Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Merck Department of Process and Analytical Chemistry, Rahway, NJ
- MP 248 **Peptide Ion Structure Investigation; From Conformational Space Sampling to Accurate CCS Calculation;** Samaneh Ghassabi Kondalaji¹; Mahdiar Khakinejad²; Stephen J. Valentine²; Amirmahdi Tafreshian²; ¹West Virginia University, Morgantown, WV; ²West Virginia University, Morgantown, WV
- MP 249 **Stability of a Transient Protein Complex in a Charged Aqueous Droplet with Variable pH;** Styliani Consta; London, ON, Canada

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- MP 250 **Selective Ion Ultraviolet Photodissociation (UVPD) Utilizing Ion Trap Resonance Excitation Modulation of Peptide and Protein Ions;** Dustin D. Holden¹; James D. Sanders¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- MP 251 **Study on the Solvent Clusters' Effect on Ionization Efficiency of Polycyclic Aromatic Hydrocarbons by (+) Atmospheric Pressure Photoionization;** Seulgidan Lee¹; Arif Ahmed¹; Sunghwan Kim¹; ¹Kyungpook National University, Daegu, South Korea
- MP 252 **Capture of Fleeting Amine Radical Cations and Elucidation of Chain Processes in Visible Light-Mediated [3+2] Annulation by Mass Spectrometry;** Yi Cai¹; Jiang Wang²; Yuexiang Zhang¹; Zhi Li¹; Hao Chen¹; Nan Zheng²; ¹Ohio University, Athens, OH; ²University of Arkansas, Fayetteville, AR
- MP 253 **REMPI and MATI Spectroscopy of Pyridine Derivatives;** Niklas Helle¹; Sascha Krüger¹; Tassilo Muskatt¹; Jürgen Grottemeyer¹; ¹Inst. f. Phys. Chem der CAU zu Kiel, Kiel

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- MP 255 **High Speed Analysis: Combining Fast GC with Time-of-Flight Mass Spectrometry for Complex Sample Analysis in Under One Minute;** Jonelle Shiel¹; Matthew Soyk²; Aviv Amirav^{3,4}; Alex Fialkov³; Viatcheslav Artaev²; ¹LECO Corporation, St. Joseph, MI; ²LECO Corporation, St. Joseph, MI; ³School of Chemistry, Tel Aviv University, Tel Aviv, Israel; ⁴Aviv Analytical Ltd, Tel Aviv, Israel
- MP 256 **GCxGC-HRMS: Combining Multidimensional GC with Ultra High Resolution Time-of-Flight Mass Spectrometry for Comprehensive Analysis of Complex Samples;** Viatcheslav Artaev¹; Scott J. Pugh²; George Tikhonov²; ¹LECO Corporation, St. Joseph, MI; ²LECO Corporation, St. Joseph, MI
- MP 257 **Development and Application of a Sensitive Analytical Method for the Analysis of Cyanobacteria-Related Off-Flavor Compounds in Water using GC-MS/MS;** Morgan Sollic¹; Benoît Barbeau¹; ¹Polytechnique Montréal - NSERC Industrial Chair on Drinking Water, Montréal, QC, Canada, Canada
- MP 258 **Improving the Chromatographic Capabilities of an Atmospheric Pressure Chemical Ionisation Source Coupled to a Gas Chromatograph;** Gareth Rhys Jones¹; David Douce¹; Richard Jarrold¹; Anthony Hesse¹; ¹Waters Wilmslow UK, Wilmslow, Cheshire
- MP 259 **Online GCMS Measurement Method using Autosampler: SPME and Purge-Trap Technique;** Jaewon Choi¹; Sung-Yun Ahn¹; Wonkyung Lee²; Il-hwan Choi¹; Yuns Kim¹; ¹Kwater, Daejeon, Daejeon; ²Euro Science, Seoul, South Korea
- MP 260 **Evaluation of Field Ionization Source Parameters Using GCxGC-FI-TOFMS for Petroleum Distillate Fractions Analysis;** Hung Anthony Pham¹; Wayne Rathbun¹; Haiyan Wang¹; Kendall Guyer¹; ¹UOP LLC, Des Plaines, IL
- MP 261 **Residual Solvents Analysis: Satisfying USP 467 Using a New Benchtop Time-of-Flight Mass Spectrometer;** Joe Binkley¹; Christina Kelly²; Lorne Fell¹; ¹LECO Corporation, Saint Joseph, MI; ²LECO Corporation, Saint Joseph, MI
- MP 262 **Japanese Lacquer Film Analysis by using Pyrolysis Comprehensive Two-Dimensional GC (Py/GCxGC) and High-Resolution TOFMS with Electron Ionization and Photoionization;** Masaaki Ubukata¹; Jun Onodera¹; Noriyasu Niimura¹; Andrew John Dane²; Yoshimi Kamiya³; ¹JEOL Ltd., Akishima, Japan; ²JEOL USA Inc., Peabody, MA; ³Tokyo Metropolitan Industrial Technology Research Institute, Akishima, Japan



- MP 263 **Estimation of Elemental Compositions for Additives in Polymers using Newly Developed EI/CI Ion Source without Venting MS**; Yukihiko Kudo¹; Riki Kltano²; Yoshiro Hiramatsu¹; Yuki Sakamoto¹; Katsuhiro Nakagawa¹; Haruhiko Mlyagawa¹; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*Shimadzu Scientific Instruments, Columbia, MD*
- MP 264 **The Analysis of All 209 PCB Isomers using GC-APCI-MS/MS at Selected Collision Energies and Correlation with Toxicity**; Jerry Hart¹; Gareth Rhys Jones²; Malcolm Clench¹; ¹*BMRC, Sheffield Hallam University, Sheffield, UK*; ²*Waters Corporation, Wilmslow, UK*
- MP 265 **Interleaving Ionisation Energy for Enhanced Confidence in the Identification of Fragrance Allergens**; Pete Grosshans¹; Natasha Spadafora¹; Matthew Edwards²; Laura McGregor¹; Chris Hall¹; Nick Bukowski¹; ¹*Makes International, Llantrisant, Cardiff*; ²*SepSolve Analytical, Peterborough, UK*
- MP 266 **Coupling of Microfabricated GC Columns with a High Pressures Ion Trap Mass Spectrometer**; Yury Desyaterik¹; John Perry¹; Tina E. Stacy¹; Jean Pierre Alarie¹; Kevin Schultze²; J. Michael Ramsey¹; ¹*UNC Chapel Hill, Chapel Hill, NC*; ²*908 Devices Inc., Boston, MA*
- MP 267 **Tandem Vacuum Ultraviolet Spectroscopy and Mass Spectrometry for Improved Identification of GC-Eluting Species**; Ian G. M. Anthony¹; Matthew R. Brantley¹; Christina A. Gaw¹; Adam R. Floyd¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*
- MP 268 **Using Low Electron Energy Automatic Tuning to Increase High Mass Sensitivity on Orbitrap GC/MS**; Xin Zheng¹; Jason Cole¹; Brody Guckenberger¹; Deven Shinholt¹; Cristian Cojocariu²; Paul Silcock²; ¹*Thermo Fisher Scientific, Austin, TX*; ²*Thermo Fisher Scientific, Runcorn, UK*
- MP 269 **Applications for a Newly Developed Miniature GC-MS System**; Kevin P. Schultze¹; James A. Roush¹; Emily E. Dunn²; Andrew C. McDowell¹; Scott E. Miller¹; ¹*908 Devices Inc., Boston, MA*; ²*Northeastern University, Boston, MA*
- MP 270 **Analysis of Pesticides and Environmental Pollutants in Essential Oil Using Multi-Platform GC/SQ, GC/ITQ and GC/Q-TOF**; Vivian Xianyu Chen¹; Kai Chen²; Bruce Quimby³; Andy Zhai¹; ¹*Agilent Technologies, Shanghai, China*; ²*Agilent Technologies, Santa Clara, CA*; ³*Agilent Technologies, Wilmington, DE*
- MP 271 **Reduction in EI Source Contamination: The Benefits of a Novel GC with an Inert Microfluidic Flow Path**; Matthew Giardina¹; Rebecca Veeneman²; ¹*Agilent Technologies, Inc., Wilmington, DE*; ²*Agilent Technologies, Inc., Wilmington, DE*
- MP 272 **Use of Methylamine PICI for Qualitative Analysis by GC/Q-TOF**; Ryo Ogasawara¹; Sadao Nakamura¹; ¹*Agilent Technologies Japan, Hachioji-shi, Tokyo*
- MP 273 **Allergens in Perfume by GC/Q-TOF with a Low Energy EI Source**; Jennifer Sanderson¹; Matthew Curtis²; ¹*Agilent Technologies, Inc., Santa Clara, CA*; ²*Agilent Technologies, Santa Clara, CA*
- MP 274 **Analysis of Sulfur Containing Compounds in Heavy Matrices using Low Energy Electron Ionization**; Matthew Curtis¹; Jennifer Sanderson²; ¹*Agilent Technologies, Santa Clara, CA*; ²*Agilent Technologies, Inc., Santa Clara, CA*
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- MP 276 **Direct Imaging and Profiling of Mycobacterium tuberculosis and Fungal Lipids within Infected Tissue Lesions by MALDI-MSI and Laser Capture Microdissection**; Brendan Prideaux¹; Landry Blanc¹; Veronique Dartois¹; ¹*PHRI, Rutgers University, Newark, NJ*
- MP 277 **Study of Changes in the Kidney's Lipid Profile in the Case of Obesity using MALDI-ToF Imaging and ESI LC-MS-MS Analysis**; Gianluca Sighinolfi¹; Daniela Cota²; Marc Bonneau¹; Jean-Marie Schmitter¹; Boutayna Rhouiri-Frih¹; ¹*CBMN, Bordeaux, France*; ²*Inserm, Bordeaux, France*
- MP 278 **Age-dependent Shift in Ganglioside Abundance Detected in Transgenic APP Rats using MALDI Imaging Mass Spectrometry**; Sarah Caughlin¹; Shikhar Maheshwari²; Ken K.-C. Yeung²; David F. Cechetto²; Shawn N. Whitehead³; ¹*Western University, London, Ontario*; ²*University of Western Ontario, London, ON, Canada*; ³*University of Western Ontario, London, ON, Canada*
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- MP 281 **Differentiating Macrophages in Atherosclerotic Plaques using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Pegah Khamsehgil-Silz¹; Florian Schnitter²; Su Hwan Kim²; Andreas H. Wagner²; Stefanie Gerbig¹; Sabine Schulz¹; Markus Hecker²; Bernhard Spengler¹; ¹*Justus Liebig University Giessen, Giessen, Germany*; ²*University of Heidelberg, Heidelberg, Germany*
- MP 282 **Imaging of Lipid Distribution in a Metastatic Breast Cancer Mouse Model**; Shelley N. Jackson¹; Ludovic Muller¹; Aurélie Roux¹; Marise Heerma van Voss²; Venu Raman²; Amina S. Woods¹; ¹*NIDA-IRP, NIH, Baltimore, MD*; ²*Johns Hopkins University School of Medicine, Baltimore, MD*
- MP 283 **High-Spatial Resolution Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging of Mouse Pancreatic Islets**; Ruichuan Yin¹; Lori Sussel²; Jennifer Kyle¹; Kristin Burnum-Johnson¹; Charles Ansong¹; Julia Laskin¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Barbara Davis Center for Diabetes, University of Colorado, Aurora, CO*
- MP 284 **Imaging Regiospecific Lipid Turnover in Mouse Brain with Desorption Electrospray Ionization Mass Spectrometry**; Richard H. Carson¹; Charlotte Lewis¹; Mercedes N. Erickson¹; Paul B. Farnsworth¹; John Price¹; ¹*Brigham Young University, Provo, UT*
- MP 285 **Alcohol Consumption during Gestation Period Alters Phosphatidylcholine and Phosphatidylethanolamine Distribution in Developing Fetal Brain**; Aafreen Kaur Bagga¹; Paige Whyte-Fagundes¹; Georg R. Zoidl¹; Demian R. Iffa¹; ¹*York University, Toronto, ON, Canada*
- MP 286 **A Multi-Center Study Using Desorption Electrospray Ionization Mass Spectrometry Imaging as A Robust Tool for Breast Cancer Diagnosis**; Jialing Zhang¹; Andréia M. Porcari²; Raquel R. Peres²; Kyana Garza¹; Jonathan Young¹; John Lin¹; Rob Tibshirani³; Geisilene R. Paiva²; Wendong Yu⁴; Chandandeep Nagi⁴; Tacey Carter⁴; Luis Z. Sarian²; Marcos N. Eberlin²; Livia S. Eberlin¹; ¹*The University of Texas, Austin, TX*; ²*State University of Campinas, Campinas, Brazil*; ³*Stanford University, Stanford, CA*; ⁴*Baylor College of Medicine, Houston, TX*
- MP 287 **Nano-DESI Imaging for Detection of oxidative stress response associated to the Neurotoxicant Paraquat Exposure in Parkinson's Like Disease Animal Model**



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- MP 288 **Tissue Mass Spectrometry Imaging Enabled Mapping of Sandhoff Biomarkers in Mouse Brain**; Walter Korfmacher¹; Cristina Silvescu¹; Hanlan Liu¹; John Marshall²; Jennifer Nietupski²; Dinesh Bangari²; Susan Ryan²; Petra Oliva²; Thomas O'Shea¹; ¹*Sanofi, Waltham, MA*; ²*Sanofi, Framingham, MA*
- MP 289 **Mass Spectrometry Imaging of Lipids in Niemann-Pick Disease C1**; Fernando Tobias¹; Abraham Abraham¹; Stephanie M Cologna¹; ¹*University of Illinois at Chicago, Chicago, IL*
- MP 290 **Molecular Characterization and Diagnosis of Endometriosis to Aid in Surgical Resection using Ambient Ionization Mass Spectrometry**; Clara Feider¹; Suzanne Ledet²; Michael T. Breen²; Livia S. Eberlin¹; ¹*University of Texas at Austin, Austin, TX*; ²*Seton Medical Center, Austin, TX*
- MP 291 **Identification of Biomarkers for Mild Traumatic Brain Injury in Tissue and Biological Fluids using DESI and PaperSpray Ionization with HRAM**; Joseph H Kennedy¹; Riya Shi²; Marcela Cruz-Haces²; Jonathan Tang²; Brian Laughlin¹; Justin Wiseman¹; ¹*Prosolia, Inc., Indianapolis, IN*; ²*Purdue University, West Lafayette, IN*
- MP 292 **MALDI-FTICR Mass Spectrometry Imaging Reveals Dysregulated Metabolites in the Brains of Zika Virus Infected Mice**; Lisa H. Cazares^{1,2}; Darci R. Smith²; Bradley Hollidge²; Xiankun Zeng²; Candace Blancett²; Tara Kenny²; Connie Schmaljohn²; Sina Bavari²; ¹*Henry M. Jackson Foundation, Frederick, MD*; ²*U.S. Army Medical Research Institute of Infectious Disease, Ft. Detrick, MD*
- MP 293 **Visualization of Aldosterone on Adrenal Frozen Sections of Primary Aldosteronism Patients**; Yuki Sugiura¹; Koshiro Nishimoto²; Shuichi Shimma³; Emi Takeo³; Makoto Suematsu¹; ¹*Keio University, Tokyo*; ²*Saitama Medical University International Medical Center, Iruma, Japan*; ³*Osaka University, Suita, Japan*
- MP 294 **High Spatial and Mass Resolution MALDI- Imaging Mass Spectrometry of Rat Optic Nerve Glial Scar Tissue**; David M. G. Anderson¹; David T. Stark²; Nathan Heath Patterson¹; Jacky M. Kwong²; Kevin L. Schey¹; Joseph Caprioli²; Richard M. Caprioli¹; ¹*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ²*Stein Eye Institute, Los Angeles, CA*
- MP 295 **MALDI-MSI Characterization of the Mesenteric Lymph Nodes during the Development of Pathophysiological Processes: An Acute Radiation Injury Model**; Claire Louise Carter¹; Kim Hankey²; Jace W Jones³; Ann M Farese³; Thomas J MacVittie²; Maureen A Kane³; ¹*University of Maryland, Baltimore, MD*; ²*University of Maryland School of Medicine, Baltimore, MD*; ³*University of Maryland School of Pharmacy, Baltimore, MD*
- MP 296 **Multi-Modal Imaging: Fusing Mass Spectrometry Imaging and Second Harmonic Generation to Understand Molecular Signatures and Collagen Alignment in Pancreatic Cancer**; Jillian Johnson¹; Adib Keikhosravi²; Catherine Pearce²; Matthew Huppert¹; Kevin Eliceiri²; Melissa Skala²; W. John Kao³; Lingjun Li^{1,4}; ¹*School of pharmacy, University of Wisconsin Madison, Madison, WI*; ²*Department of Biomedical Engineering, University of Wisconsin-Madison, Madison, WI*; ³*President's Office, The University of Hong Kong, Pokfulam, Hong Kong*; ⁴*Department of chemistry, University of Wisconsin Madison, Madison, WI*
- MP 297 **Exploration of Desorption Electrospray Ionization (DESI) and Touch Spray (TS) Mass Spectrometry for Squamous Cell Carcinoma (SCC) Diagnosis and Prognosis**; Cedric DHue¹; Michael Moore²; Don-John Summerlin³; Alan Jarmusch⁴; R. Graham Cooks⁵; ¹, *West Lafayette, IN*; ²*University of California, Davis, Davis, CA*; ³*Indiana University-Purdue University Indianapolis, Indianapolis, IN*; ⁴*University of California, San Diego, San Diego, CA*; ⁵*Purdue University, West Lafayette, IN*
- MP 298 **Tissue Microarrays Analysis using DESI-MSI**; Anna K Mróz¹; Luisa Doria¹; James McKenzie¹; Francesca Rosini¹; Hiromi Kudo¹; Zoltan Takats¹; Renata Soares¹; ¹*Imperial College London, London, UK*
- MP 299 **Co-localization of N-glycan and Peptide Tumor Clusters by MALDI-FTICR Mass Spectrometry Imaging of FFPE Tissues**; Kim Norris-Caneda¹; Alyson Black¹; Peggi M Angel¹; Richard R Drake¹; ¹*Medical University of South Carolina, Charleston, SC*
- MP 300 **Mapping the Similarities and Differences in the N-glycomes of Twenty Tumor Types using MALDI-FTICR Mass Spectrometry Imaging**; Richard R Drake¹; Kacey Talbot¹; Fred David¹; Kim Norris-Caneda¹; Evelyn Bruner¹; Anand Mehta¹; Peggi M Angel¹; ¹*Medical University of South Carolina, Charleston, SC*
- MP 301 **N-Glycan Changes in the Human Aortic Valve during Development and Disease by Imaging Mass Spectrometry**; Kacey Talbot¹; Aaron Reed¹; H. Scott Baldwin²; David Bichell³; Yan Ru Su²; Richard R Drake¹; Peggi M. Angel¹; ¹*Medical University of South Carolina, Charleston, SC*; ²*Vanderbilt University School of Medicine, Nashville, TN*; ³*Vanderbilt University Medical Center, Nashville, TN*
- MP 302 **Imaging Lipid and Protein Changes in Human Diabetic Kidney by MALDI Mass Spectrometry**; Michael Tuck¹; Michelle L Reyzer¹; Nathan Heath Patterson¹; Haichun Yang¹; Raymond Harris¹; Agnes B Fogo¹; Richard M. Caprioli¹; ¹*Vanderbilt University, Nashville, TN*
- MP 303 **High Performance Imaging MS and Data-Driven Image Fusion to Characterize Colon Structures and Immune Cell Infiltrates at the Protein Level**; Martina Marchetti-Deschmann¹; Boone M. Prentice²; Raf Van de Plas^{3,4}; Matthias Holzlechner¹; Rudolf Oehler⁵; Jeffrey M. Spraggins⁴; Richard M. Caprioli⁴; ¹*Vienna University of Technology, Vienna, Vienna*; ²*Mass Spectrometry Research Center, Department of Biochemistry, Vanderbilt University, Nashville, TN*; ³*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*; ⁴*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ⁵*Medical University of Vienna, Vienna, Austria*
- MP 304 **MALDI Mass Spectrometry Imaging Investigation of Chemico-Spatial Composition of the Parathyroid Gland**; Qiyao Li¹; Stanislav S Rubakhin¹; Robyn E Ellerbrock¹; Brian M Aldridge¹; Adam C Puche²; Iris Lindberg²; Jonathan V Sweedler¹; ¹*University of Illinois at Urbana Champaign, Urbana, IL*; ²*University of Maryland School of Medicine, Baltimore, MD*
- MP 305 **Discerning the Primary Carcinoma in Different Malignant Peritoneal Effusions by Imaging Mass Spectrometry**; Kristina Schwamborn¹; Wilko Weichert¹; Gregor Weirich¹; Richard M. Caprioli²; ¹*Technical University Munich, Munich*; ²*Vanderbilt University, Nashville, TN*
- MP 306 **Top-down Neuropeptide MALDI Imaging MS on FFPE Sections with High Mass Resolution and MS/MS Capabilities: Towards True "Mass Spectrometry Histochemistry"**; Peter D. Verhaert¹; Shane R. Ellis²; Martin R. L. Paine²; Dan Maloney³; Ron MA Heeren²; ¹*Delft University of Technology, DELFT, Europe*; ²*Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands*; ³*Bioinformatics Solutions Inc, Waterloo, ON, Canada*
- MP 307 **A Combined Approach to Improve Identification of Protein Markers of Sinusoidal Obstruction Syndrome by Mass Spectrometry Imaging**; Pierre-Maxence Vaysse^{1,2}; Junfang Zhao²; Celien P. Vreuls³; Benjamin Balluff¹; ¹, *West Lafayette, IN*; ²*University of California, Davis, Davis, CA*; ³*Indiana University-Purdue University Indianapolis, Indianapolis, IN*; ⁴*University of California, San Diego, San Diego, CA*; ⁵*Purdue University, West Lafayette, IN*



Zita Soons²; Ronny Mohren¹; Sander S. Rensen²; Steven W.M. Olde Damink²; Ron M. A. Heeren¹; Tiffany Porta¹; ¹Maastricht University, Maastricht Multimodal Molecular Imaging (M4I) institute, Maastricht, Netherlands; ²Maastricht University Medical Center +, Department of General Surgery, Maastricht, Netherlands; ³Department of Pathology, Amphia Hospital, Breda, Netherlands

- MP 308 **Visualizing Molecular Remodeling in a Mouse Model of Preterm Labor via MALDI Imaging Mass Spectrometry;** Michelle L Reyzer¹; Nathan Heath Patterson¹; Michael Tuck¹; M Lisa Manier¹; Naoko Brown¹; Christine O'Brien¹; Mike F Robuck¹; Jennifer L Herington¹; Jeff Reese¹; Richard M. Caprioli¹; ¹Vanderbilt University, Nashville, TN
- MP 309 **Bead-Array Mass Spectrometry Imaging for Drug Discovery and Multiplex Diagnostic Biomarker Detection;** Gargey B. Yagnik¹; Mark J. Lim¹; Kenneth J. Rothschild¹; ¹AmberGen, Inc., Watertown, MA

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- MP 310 **Param-Medic Breathes New Life into MS/MS Database Search by Optimizing Parameter Settings;** Damon May¹; Kaipo Tamura¹; William S Noble^{1,2}; ¹University of Washington Genome Sciences, Seattle, WA; ²University of Washington Computer Science and Engineering, Seattle, WA
- MP 311 **Modeling EThcD Spectrum with Linear Discriminant Function for Peptide Identification;** Lei Xin¹; Wen Zhang¹; Baozhen Shan¹; ¹Bioinformatics Solutions Inc, Waterloo, ON, Canada
- MP 312 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data;** Luis Mendoza¹; David Shteynberg²; Michael R. Hoopmann²; Henry Lam³; Jimmy K Eng⁴; Eric W. Deutsch²; Robert L. Moritz²; ¹Institute For Systems Biology, Seattle, WA; ²Institute for Systems Biology, Seattle, WA; ³Hong Kong University of Science and Technology, Hong Kong, China; ⁴University of Washington, Seattle, WA
- MP 313 **Protein Identification without Peptide Identification;** Jamie Sherman¹; Stephen Tate²; ¹SCIEX, Concord, ON, Canada; ²SCIEX, Concord, ON, Canada
- MP 314 **Analysis of Protein-Peptide Bipartite Networks with ProteinClusterQuant for the Accurate Quantification of Proteoforms in Complex Protein Samples;** Salvador Martínez-Bartolomé¹; Casimir Bamberguer¹; Miranda Montgomery¹; Sandra Pankow¹; John R. Yates III¹; ¹The Scripps Research Institute, La Jolla, CA
- MP 315 **Using Fragmentation Specificity and Coverage to Improve Mass Spectrometry Based Peptide Identification;** Zhi Li¹; Xuya Wang¹; Sisi Ma²; Kelly V. Ruggles¹; David Fenyó¹; ¹New York University School of Medicine, New York, NY; ²University of Minnesota, St. Paul, MN
- MP 316 **An Efficient Filtering Algorithm for Proteoform Identification by Top-Down Tandem Mass Spectra;** Runmin Yang^{1,2}; Daming Zhu¹; Xiaowen Liu^{2,3}; ¹Department of Computer Science and Technology, Shandong University, Jinan, China; ²Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN
- MP 317 **An Algorithm for the Annotation of PTMs using Isotopic Structure Data;** Michał Startek¹; Mateusz Krzysztof Łacki¹; Anna Gambin¹; ¹University of Warsaw, Warsaw, Mazowieckie
- MP 318 **Methods for FDR Estimation in High Mass Accuracy Peptide Spectral Library Searches;** Zheng Zhang¹; Yuri A. Mirokhin¹; Dmitrii V. Tchekhovskoi¹; Sanford P. Markey¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD

- MP 319 **The Hybrid Search: New Accurate Mass Spectral Library Search Software for Discovery of Modifications in Proteomics;** Meghan Burke¹; Yuri A. Mirokhin¹; Dmitrii V. Tchekhovskoi¹; Sanford P. Markey¹; Jenny Heidbrink Thompson²; Christopher Larkin²; Stephen E. Stein³; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²MedImmune LLC, Gaithersburg, Maryland; ³National Institute of Standards and Technology, Gaithersburg, MD
- MP 320 **Confidence Assignment for Mass Spectrometry Based Peptide Identifications via the Extreme Value Distribution;** Gelio Alves¹; Aleksey Ogurtsov¹; Yi-Kuo Yu¹; ¹National Center for Biotechnology Information, NLM, Bethesda, MD
- MP 321 **Controlling False Discovery Rate in Accumulated Public Proteome Dataset;** Akiyasu C. Yoshizawa¹; Tsuyoshi Tabata²; Yuki Moriya³; Shin Kawano³; Shujiro Okuda⁴; Yu Watanabe⁴; Tadashi Yamamoto⁵; Masaki Matsumoto⁶; Tomoyo Takami⁶; Daiki Kobayashi⁷; Norie Araki⁷; Naoyuki Sugiyama²; Satoshi Tanaka⁸; Susumu Goto³; Yasushi Ishihama²; ¹Bioinformatics Center, Institute for Chemical Research, Kyoto University, Uji, Japan; ²Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ³Database Center for Life Science, Joint Support-Center for Data Science Research, Research Organization of Information and Systems, Kashiwa, Japan; ⁴Niigata University Graduate School of Medical and Dental Sciences, Niigata, Japan; ⁵Biofluid Biomarker Center, Institute for Research Collaboration and Promotion, Niigata University, Niigata, Japan; ⁶Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; ⁷Graduate School of Medical Sciences, Kumamoto University, Kumamoto, Japan; ⁸Trans-IT, Kaminokawa, Japan
- MP 322 **Leveraging Time Series LC-MS/MS Experiments to Explore Unidentified Peptide Sequencing Data;** Armin G. Geiger^{1,2}; Richard J. Giannone¹; Paul E. Abraham¹; Daniel A. Jacobson¹; ¹Oak Ridge National Lab, Oak Ridge, TN; ²Bredesen Center for Interdisciplinary Research and Graduate Education, Knoxville, TN
- MP 323 **Predicting Acquisition Dependent Peptide Fragmentation Rules using a Single Deep Neural Network;** Siegfried Gessulat^{1,2}; Mathias Wilhelm¹; Daniel P. Zolg¹; Tobias K. Schmidt¹; Patroklos Samaras¹; Peng Yu¹; Judith Schlegel³; Hans-Christian Ehrlich²; Stephan Aiche²; Bernhard Kuster^{1,4,5}; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²SAP SE, Potsdam, Germany; ³SAP SE, Walldorf, Germany; ⁴Center for Integrated Protein Science Munich, Freising, Germany; ⁵Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany
- MP 324 **Evaluating the Impact of Multiple Search Engines and De-novo Sequencing Algorithms for Obtaining Deeper Proteome Coverage in Complex Environmental Samples;** Ramsunder Iyer^{1,2}; Robert L. Hettich²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- MP 325 **Increased Throughput and Accuracy in Host Cell Protein Quantitation using Spectral Library Searches;** Martha Stapels¹; Michelle Busch¹; John Ray¹; Ian Reah²; Steven Anderson²; Ian Morns²; ¹Sanofi, Framingham, MA; ²Waters Corporation, Newcastle upon Tyne, UK
- MP 326 **Combining Different Search Engines and Data Processing Tools for Proteomics Identification and Quantitation;** Ying Zhang¹; Zhihui Wen¹; Mike Washburn¹; Laurence Florens¹; ¹Stowers Institute for Medical Research, Kansas City, MO
- MP 327 **Mass-MetaSite and WebMetabase: Tools for the Identification and Prediction of Protease Cleavage Sites in Peptide Drugs;** Ismael Zamora^{1,2}; Tatiana Radchenko^{1,2}; Christopher Kochansky³; Alison Bateman³; Andreas Brink⁴;



MONDAY POSTERS

- Fabien Fontaine²; Luca Morettoni⁵; ¹Universitat Pompeu Fabra, Barcelona, Spain; ²Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; ³Merck & Co., West Point, PA; ⁴Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland; ⁵Molecular Discovery, London, UK
- MP 328 **Systematic Evaluation of Filtering Algorithms for the Identification of Proteoforms with Multiple Alterations using Top-Down Tandem Mass Spectrometry**; Qiang Kou¹; Si Wu²; Xiaowen Liu^{1,3}; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²University of Oklahoma, Norman, OK; ³Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN
- MP 329 **Assembling the Community-Scale Discoverable Human Proteome**; Mingxun Wang¹; Jian Wang¹; Nuno Bandeira^{1,2}; ¹UCSD, La Jolla, CA; ²Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA
- MP 330 **Pulsar: A Search Engine Integrated into Spectronaut using Dynamic PSM Stratification**; Lynn Verbeke¹; Oliver M. Bernhardt¹; Tejas Gandhi¹; Roland Bruderer¹; Lukas Reiter¹; ¹Biognosys, Schlieren, Zurich
- MP 331 **Workflow for Simultaneous Biotherapeutic Peptide Mapping and Host Cell Protein Analysis Utilizing In-silico Peptide Monitoring**; Heather Anderson¹; Alyssa Spitznogle¹; Christopher A Bolcato¹; Matthew J Powell¹; K. Ilker Sen²; St John skilton²; Eric Carlson²; Matthew D Maust¹; ¹Protea Biosciences, Morgantown, WV; ²Protein Metrics Inc., San Carlos, CA
- MP 332 **Identification of Regulatory miRNAs Associated with Ethanol-Induced Microglial Activation Using Integrated Proteomic and Transcriptomic Approaches**; Brandi Cook¹; Robert Hill²; Dale Chaput²; Bin Liu³; Stanley M. Stevens²; ¹University of South Florida, Tampa, Florida; ²University of South Florida, Tampa, FL; ³University of Florida, Department of Chemistry, Gainesville, FL
- MP 333 **BUPID-XL for Identification of Cross-linked Peptides in LC-MS/MS Data**; Christian F. Heckendorf¹; Deborah R. Leon¹; Alex J. McDonald¹; Catherine E. Costello¹; Mark E. McComb¹; ¹Boston University School of Medicine, Boston, MA
- MP 334 **Towards a m/z Unlimited Algorithm for Peptide and Protein Structure Elucidation**; Fabien Fontaine^{1,2}; Ismael Zamora^{1,3}; Christopher Kochansky⁴; ¹Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; ²Molecular Discovery, London, UK; ³Pompeu Fabra University, Barcelona, Spain; ⁴Merck & Co., West Point, PA
- MP 335 **Identifying Co-Eluting Peptides using MS Amanda and Elutator**; Viktoria Dorfer¹; Sergey Maltsev²; Stephan Winkler¹; Karl Mechtler^{2,3}; ¹University of Applied Sciences Upper Austria, Hagenberg, AUT; ²Research Institute of Molecular Pathology (IMP), Vienna, Austria; ³Institute of Molecular Biotechnology, Vienna, Austria
- MP 336 **PeptidePicker Version 2: Selecting Suitable Proteotypic Peptides for Targeted Proteomics Experiments**; Yassene Mohammed^{1,2}; Pallab Bhowmick¹; Christoph H. Borchers^{1,3,4}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Center for Proteomics and Metabolomics, Leiden University, Netherlands; ³Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁴Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada
- MP 337 **CONSTAND++: An Efficient Method for Quantitative Proteomics Data Analysis**; Joris Van Houtven¹; Evelynne Maes²; Kris Laukens³; Geert Baggerman^{3,4}; Jef Hooyberghs⁴; Dirk Valkenborg^{1,3}; ¹Hasselt University, Diepenbeek, Limburg; ²AgResearch, Christchurch, New Zealand; ³University of Antwerp, Antwerp, Belgium; ⁴VITO, Mol, Belgium
- MP 338 **A Novel Machine Learning Approach to Calculate FDR for label Free Quantification**; Johannes Doblmann¹; Frederico Dusberger¹; Richard Imre¹; Otto Hudecz²; David M Hollenstein³; Karl Mechtler^{1,2}; Gerhard Duernberger^{1,2,4}; ¹IMP, Vienna, Vienna; ²IMBA - Institute of Molecular Biotechnology, Vienna, Austria; ³MFPL-Max F. Perutz Laboratories, Vienna, Austria; ⁴GMI - Gregor Mendel Institute for Molecular Plant Biology, Vienna, Austria
- MP 339 **Building Peptide Tandem Mass Spectral Libraries of Consensus Spectra**; Sergey L. Sheetlin¹; Dmitrii V. Tchekhovskoi¹; Yuri A. Mirokhin¹; Stephen E. Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- MP 340 **DeltaMass: Analysis and Viewer Software for Examining Wide Precursor Window Search Results in Proteomics**; Dmitry M. Avtonomov¹; Andy Kong¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- MP 341 **Improvements to Protein Prospector's MS-Viewer**; Peter R Baker¹; Carolyn Chitty²; Robert J Chalkley²; ¹UCSF, Rokietnica; ²UCSF, San Francisco, CA

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- MP 342 **Identification of an Unknown Biocide by Vapor Atmospheric Pressure Chemical Ionization (vAPCI) and Compact Mass Spectrometry (CMS)**; Daniel Eikel¹; Simon J Prosser¹; ¹Advion Inc., Ithaca, NY
- MP 343 **On-paper Sample Handling for Bottom-up Protein Analysis**; Oeystein Skjaervoe¹; Trine Grønhaug Halvorsen¹; Léon Reubsaet¹; ¹School of Pharmacy, University of Oslo, Oslo, Norway
- MP 344 **Molecular-beam Mass Spectrometric and Numerical Investigation of the Intrusive Flame Sampling Effect on Premixed Low-Pressure Flame Structure**; Yasin Karakaya¹; Lei Deng¹; Irenäus Wlokas¹; Martin Höner¹; Tina Kasper¹; ¹University of Duisburg-Essen, Duisburg, Germany
- MP 345 **Sample Flow Rate Scan in Mass Spectrometry**; Gurpur Rakesh D. Prabhu¹; Pawel L. Urban¹; ¹National Chiao Tung University, Hsinchu, Taiwan
- MP 346 **Glove Box Compatible Sampling and Characterization of Reactive Compounds by LIFDI MS**; Mathias Linden¹; H. Bernhard Linden¹; ¹Linden CMS, Weyhe, Niedersachsen
- MP 347 **Polymer Inclusion Membrane use with Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS): Robust Membranes with Superior Analytical Performance Characteristics**; Gregory W. Vandergrift^{1,2}; Erik T. Krogh^{1,2}; Christopher G. Gill^{1,2,3,4}; ¹Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada; ²Chemistry Department, University of Victoria, Victoria, BC, Canada; ³Chemistry Department, Simon Fraser University, Burnaby, BC, Canada; ⁴University of Washington, Department of Chemistry, Seattle, WA
- MP 348 **Analytical Tool for the Study of Collection Efficiency of Explosives from Surfaces**; Vladimir Romanov¹; Steven Watt¹; Thomas Hagerty¹; Hartwig Schmidt¹; Stefan Lukow¹; ¹Morpho Detection, Andover, MA
- MP 349 **Accessing High Performance Microflow on a Chip-Based Platform**; Helena Svobodova¹; Aaron Dewberry¹; Amanda Berg¹; Mike S. Lee²; Gary Valaskovic¹; ¹New Objective, Woburn, MA; ²Milestone Development Services, Inc., Newtown, PA
- MP 350 **Open-Port Probe Sampling Interface for the Direct Coupling of Solid-Phase Microextraction to Atmospheric Pressure Ionization Mass Spectrometry**; Chang Liu¹; Germán Gómez-Ríos²; Marcos Tascon²; Bradley B Schneider¹; Nathaly Reyes-Garcés²; Don W Arnold³; Thomas R. Covey¹; Janusz Pawliszyn²; ¹SCIEX, Concord, ON, Canada; ²University of Waterloo, Waterloo, Ontario; ³SCIEX, Redwood City, CA



- MP 351 **Front-end Developments for Trace Analyte Collection, Desorption, and Ionization of Vapor and Particulate Species;** Thomas P. Forbes¹; Matthew Staymates¹; Edward Sisco¹; ¹*National Institute of Standards and Technology, Gaithersburg, MD*
- MP 352 **High-Throughput Mass Spectrometry: Direct Acoustic Ionization for Sub-Second Sample Processing in Biochemical Screens;** Lucien Ghislain¹; Martin Bachman²; Ian Sinclair²; Jonathan Wingfield³; Daniel Addison²; Eric Hall¹; Rick Stearns¹; Lars Majlof¹; Richard Ellson¹; Gareth Rhys Jones⁴; Emmy Hoyes⁴; Steven Derek Pringle⁴; Sammy Datwani¹; ¹*Labcyte Inc, Sunnyvale, CA*; ²*AstraZeneca R&D, Alderley Park, UK*; ³*Astrazeneca, Cambridge, UK*; ⁴*Waters Corporation, Wilmslow, UK*
- MP 353 **The T-probe: A Novel Device for Rapid MS Analysis of Non-Adherent Live Single Cells;** Yanlin Zhu¹; Renmeng Liu¹; Zhibo Yang¹; ¹*The University of Oklahoma, Norman, OK*
- MP 354 **High-throughput (sub-2.5 second) Direct Injection using a Modified RapidFire 365 HTMS System;** Peter Rye¹; Arrin Katz²; William LaMar²; Can Ozbal²; ¹*Agilent, Lexington, MA*; ²*Pure Honey Technologies, Billerica, MA*
- MP 355 **Development of a Mass Spectrometry Cartridge for Plasma Protein Analysis with integrated Antibody Column and Spray Substrate;** Chengsen Zhang¹; Nicholas E. Manicke¹; ¹*Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- MP 356 **Polymer-Coated Capillary Sampler for Direct Mass Spectrometry Quantitation of Fatty Acids in Biofluids;** Wenpeng Zhang^{1,2,3}; Spencer Chiang¹; Yu Xia²; Zheng Ouyang^{1,2,3}; ¹*Weldon School of Biomedical Engineering, Purdue University, West Lafayette, Indiana*; ²*Department of Chemistry, Purdue University, West Lafayette, IN*; ³*Tsinghua University, Beijing, Beijing*
- MP 357 **Robotic Surface Analysis Mass Spectrometry (RoSA-MS);** Anyin Li¹; Martin R. L. Paine¹; Rachel V Stryffeler¹; Jason Wu¹; Stephen Zambrzycki¹; Jake Huckaby²; Chu-yin Change²; Manoj Kumar²; Piyoosh Mukhija²; Alexander S Lambert¹; Ruffin J White¹; Henrik I Christensen¹; Facundo M Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Energid, Cambridge, MA*
- MP 358 **Droplet Based Sampling of RNA Hydrolysates by Induction Based Fluidics;** Robert Ross¹; Manasses Jora¹; Andrew D. Sauter III²; Drew Sauter²; Patrick A. Limbach¹; ¹*University of Cincinnati, Cincinnati, OH*; ²*Nanoliter, LLC, Henderson, NV*
- MP 359 **Atomic Force Microscope Mediated Thermal Microsampling with Atmospheric Pressure Temperature Ramped Thermal Desorption/Ionization – Mass Spectrometry Analysis;** William D. Hoffmann¹; Vilmos Kertesz¹; Gary J. Van Berkel¹; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*
- MP 360 **Ambient Submicron Sampling of Biological Samples by Combining AFM with MS;** Jonathan Brauer; *Anasys Instruments, Santa Barbara, CA*
- MP 361 **Programmable Stage for Fluorescence-Guided Atmospheric Pressure Mass Spectrometry Imaging of Frozen Tissue Sections by Laser Ablation Electrospray Ionization;** Rikkita Khattar¹; Sylwia A Stopka¹; Beverly J Agtuca²; Christopher R Anderton³; David W. Koppelaar³; Ljiljana Pasa-Tolic³; Gary Stacey²; Akos Vertes¹; ¹*George Washington University, Washington, DC*; ²*University of Missouri, Columbia, MO*; ³*Pacific Northwest National Laboratory, Richland, WA*
- MP 362 **Liquid Chromatography-Plasma Assisted Reaction Chemical Ionization Mass Spectrometry for the Analysis of Chlorinated Compounds;** Joseph Lesniewski¹; Kunyu Zheng¹; William McMahon¹; Hamid Badiei²; Heng Keang Lim³; Kaveh Jorabchi¹; ¹*Georgetown Univ., Washington, DC*; ²*PerkinElmer Inc, Shelton, CT*; ³*Janssen Research&Development, Spring House, PA*
- MP 363 **Application of an Acoustic Interface for Ultra-High-Throughput Mass Spectrometry in Drug Discovery;** ian Sinclair¹; Martin Bachman²; Jonathan Wingfield³; mattias rohman⁴; Lucien Ghislain⁵; Eric Hall⁵; Gareth Rhys Jones⁶; Michael Morris⁶; Richard Ellson⁵; Rick Stearns⁵; ¹*AstraZeneca, macclesfield, Cheshire*; ²*AstraZeneca R&D, Alderley Park, UK*; ³*Astrazeneca, Cambridge, UK*; ⁴*Astrazeneca, Mölndal, Mölndal*; ⁵*Labcyte Inc, Sunnyvale, CA*; ⁶*Waters Corporation, Wilmslow, UK*
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- MP 364 **Variable-velocity Traveling-wave Ion Mobility Separation Enhances Peak Capacity for Data-independent Acquisition Proteomics;** Sarah E. Haynes¹; Daniel A. Polasky¹; Sugyan M. Dixit¹; Jaimeen D. Majmudar¹; Brandon T. Ruotolo¹; Brent R. Martin¹; ¹*University of Michigan, Ann Arbor, MI*
- MP 365 **Impact of Ion Focusing Parameters on Transmission and Fragmentation of Coordination Driven Self-Assembly Product Ions;** Christopher S. Mallis¹; Manik L. Saha²; Peter J. Stang²; David H. Russell¹; ¹*Texas A&M University, College Station, TX*; ²*University of Utah, Salt Lake City, UT*
- MP 366 **Simulation of a Novel Annular Geometry Ion Mobility Trap and Separation Device with High Space Charge Capacity;** David Langridge¹; Martin Green¹; Kevin Giles¹; ¹*Waters Corporation, Wilmslow, UK*
- MP 367 **Measuring Precise Collision Cross Section Values from Liquid Chromatography Ion Mobility Tandem Mass Spectrometry Experiments;** Charles M. Nichols¹; Sarah M. Stow²; Jaqueline A. Picache¹; Jody C. May¹; Stacy D. Sherrod¹; John Fjeldsted²; John A. McLean¹; ¹*Vanderbilt University, Nashville, TN*; ²*Agilent Technologies, Santa Clara, CA*
- MP 368 **Ion Separation in Air Using a 3D Printed Ion Mobility Spectrometer;** Adam Hollerbach¹; Zane Baird²; Graham Cooks¹; ¹*Purdue University, West Lafayette, IN*; ²*Present address: Indiana Biosciences Research Institute, Indianapolis, IN*
- MP 369 **Ion Mobility Support in a Novel Compound-Centric Database and Accurate Mass Spectral Library;** Emma E Rennie¹; Kristina L Milkovich¹; Norton Kitagawa¹; Mahsan Miladi¹; Crystal K Cody¹; Stephen Madden¹; Nagapadmini Pavuluri¹; John C Fjeldsted¹; ¹*Agilent Technologies Inc., Santa Clara, CA*
- MP 370 **Quadrupole Wide Band Isolation Directed by Ion Mobility Drift Separation in Metabolomics Experiments;** Teresa Mairinger¹; Ruwan Kurulugama²; Tim Causon¹; George Stafford³; John Fjeldsted³; Stephan Hann¹; ¹*University of Natural Resources and Life Sciences - BOKU, Vienna, Austria*; ²*Agilent Technologies Inc., Santa Clara, CA*; ³*Agilent Technologies, Inc., Santa Clara, CA*
- MP 371 **Synchronizing Ion Mobility with Quadrupole Mass Filtering for Highly Efficient Background Removal during Acquisition for Metabolite Identification;** Jayne Kirk¹; Darren Hewitt¹; Martin Palmer¹; Jason wildgoose¹; Mark Wrona²; ¹*Waters Corp., Wilmslow, UK*; ²*Waters Corp, Milford, MA*
- MP 372 **The Use of SelexION to Increase Sensitivity for Trace Level Analysis of Small Molecules;** Christopher Borton¹; Paul C. Winkler¹; Jay Jones²; ¹*SCIEX, Framingham, MA*; ²*BASF, Research Triangle Park, NC*
- MP 373 **Building a Collision Cross Section Library of Pharmaceutical Drugs using an IMS QToF Platform ;** Yun Alelyunas¹; Kerri Smith²; Russell Mortishire-Smith²; Mark D. Wrona²; Nigel Ewing²; ¹*Milford, MA*; ²*Waters Corp, Milford, MA*



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- MP 374 **Development of a SUPER SLIM TWIM-MS Application Platform for Multi-Omics Analysis;** Christopher D. Chouinard¹; Ian K Webb¹; Spencer A Prost¹; Yehia M Ibrahim¹; Liulin Deng¹; Xueyun Y Zheng¹; Randolph V Norheim¹; Colby E Schimelfenig¹; Erin S Baker¹; RICHARD D. SMITH¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- MP 375 **Influence of Ionization Source Conditions on Protomer, or Deprotomer Ratios of Multifunctional Gaseous Ions Demonstrated by Ion Mobility Mass Spectrometry;** Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- MP 376 **High-throughput, Charge-multiplexed Collision-induced Unfolding Measurements for Rapid Biotherapeutic Analysis;** Joseph D Eschweiler¹; Ruwan Kurulugama²; John Fjeldsted²; Brandon T Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Agilent Technologies, Santa Clara, CA*
- MP 377 **Characterization of the Interaction Between microRNA 122 and Hepatitis C Viral RNA;** Cesar Masitas¹; Jonathan Trinidad¹; ¹*Indiana University Bloomington, Bloomington, IN*
- MP 378 **Separation of Isobaric Phospholipids and Fatty Acids Derived from Murine Adipose Tissue using Ion Mobility Coupled with High-Resolution Mass Spectrometry;** Christine Hinz¹; Sonia Liggi¹; Julia Denes¹; Antonio Murgia^{1,2}; Zoe Hall¹; Ke-di Liu¹; John Fjeldsted³; Julian L. Griffin¹; ¹*University of Cambridge, Cambridge, UK*; ²*Università degli Studi di Cagliari, Cagliari, Italy*; ³*Agilent Technologies, Santa Clara, CA*
- MP 379 **Extractive Electrospray Ionization Coupled to Atmospheric Pressure DTIMS-MS for Real-Time Analysis of Aerosols;** Paul S. Soma¹; Kenneth D. Swanson¹; Gary L. Glish¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MP 380 **Non-Enzymatic Stepwise Degradation of Substance P Measured by Hybrid IMS-MS;** Christopher R. P. Conant¹; Daniel R Fuller¹; Alison E Holliday²; David H Russell³; David E Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*; ²*Moravian College, Bethlehem, Pennsylvania*; ³*Texas A&M University, College Station, TX*
- MP 381 **Evidence for a Globule to Helix Gas-Phase Transition in an α -Synuclein Peptide Segment;** Goran Tumbic¹; Michael Przybylski²; David E Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*; ²*Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany*
- MP 382 **Examining the Structural Influence of Site Specific Phosphorylation by Ion Mobility-Mass Spectrometry;** Rebecca S. Glaskin¹; Caroline S. Chu²; ¹*Agilent Technologies, Inc., Wilmington, DE*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- MP 383 **Large Scale Collision Cross Section (CCS) Profiling of Endogenous Neuropeptides by Ion Mobility Mass Spectrometry;** Zichuan Tian¹; Zhengwei Chen²; Matthew Glover³; Qingwen Cao⁴; Lingjun Li^{4,5}; ¹*Madison, WI*; ²*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*; ³*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; ⁴*Department of chemistry, University of Wisconsin Madison, Madison, WI*; ⁵*School of pharmacy, University of Wisconsin Madison, Madison, WI*
- MP 384 **Simultaneous Tracking of Individual Protein Stabilities in a Mixture by Ion Mobility Spectrometry-Mass Spectrometry;** Kyle Buckley¹; Tarick El-Baba¹; Daniel W Woodall¹; David E Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*
- MP 385 **Assessment of Dimeric Metal-Glycan Adducts via Isotopic Labeling and Ion Mobility-Mass Spectrometry;** Kelsey A. Morrison¹; Brad K. Bendiak²; Brian Clowers¹;

- ¹*Washington State University, Pullman, WA*; ²*University of Colorado Health Sciences Center, Aurora, CO*
- MP 386 **Visualizing and Conceptualizing Highly-Dimensional Metabolomics Data from LC-IM-MS/MS Analysis;** Jaqueline A. Picache¹; Charles M. Nichols¹; John C. Fjeldsted²; Stacy D. Sherrod¹; Jody C. May¹; John A. McLean¹; ¹*Vanderbilt University, Nashville, TN*; ²*Agilent Technologies Inc., Santa Clara, CA*
- MP 387 **Probing Supramolecular Assembly Processes by Ion Mobility Mass Spectrometry;** Kevin J Endres¹; George R Newkome¹; Chrys Wesdemiotis¹; ¹*The University of Akron, Akron, OH*
- MP 388 **Structural Database of Secondary Metabolites: Conformational Mapping using Ion Mobility-Mass Spectrometry as a Tool for Natural Product Discovery;** Andrzej Balinski¹; John A. McLean²; Jody C. May²; Brian O. Bachmann²; Sarah M. Stow³; ¹*Vanderbilt University, Nashville, TN*; ²*Vanderbilt University, Nashville, TN*; ³*Agilent Technologies Inc., Santa Clara, CA*
- MP 389 **Differential Analysis of 4-dimensional LC-IMS-MS Data in the Analysis of Complex Samples;** Niels Goedecke¹; Peter Sander¹; Sven Meyer¹; Klaus Meyer¹; ¹*Bruker Daltonik GmbH, Bremen, Germany*

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- MP 390 **SCX Contamination: A New Class of Pan-Assay Interference Compounds (PAIS)?;** Kenneth Roth¹; Phillip Sanders¹; Brandon Margolis¹; ¹*Eli Lilly & Co., Indianapolis, IN*
- MP 391 **Analysis of Commercially Available Beta-Glucuronidase Enzymes and Optimum Hydrolysis Conditions in Urine for Licit and Illicit Drugs using In-Well Hydrolysis;** Jillian Neifeld¹; Dan Menasco¹; Stephanie J Marin¹; Bruce Kempf¹; Helen Lodder²; Alan Edgington²; Adam Senior²; Paul Roberts²; Lee Williams²; Elena Gairloch¹; Claire Desbrow²; Steve Jordan²; ¹*Biotage, Charlotte, NC*; ²*Biotage GB Limited, Cardiff*
- MP 392 **Fractionation of Whole Gut Lavage Fluid by Affinity Immunoglobulin Alpha Depletion for Increased Proteomic Coverage;** Joseph Otto¹; Jana M Rucker^{1,2}; Lewis K. Pannell¹; ¹*Mitchell Cancer Inst, Mobile, AL*; ²*Mississippi Gulf Coast Community College, Gulfport, MS*
- MP 393 **Evaluation of Recombinant, Chemically Treated Trypsin in Proteomics and Protein Characterization Assays;** Nicolas Caffarelli¹; Judy Boland¹; Jeff Turner¹; Gordon Nicol¹; Amber Henry¹; Kevin Ray¹; ¹*MilliporeSigma, St. Louis, MO*
- MP 394 **Factors Effecting the Quality of FASP-prepared Proteomics Samples;** Shekufeh Zareian¹; Michael J Sweredoski¹; Sonja Hess¹; Annie Moradian¹; ¹*Caltech, Pasadena, CA*
- MP 395 **Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid using a Novel Lipid Removing Sorbent and LC/MSMS;** Joan Stevens¹; Xiaomi Xu¹; Tarun Anumol¹; Limian Zhao¹; ¹*Agilent Technologies, Inc., Wilmington, DE*
- MP 396 **Automated Peptide Desalting using Dispersive Pipette Extraction Tips for Increased Protein Identifications;** Sunil Hwang¹; Todd Mullis¹; Michael Mouridian²; Andrew Lee¹; ¹*IMCS, Columbia, South Carolina*; ²*Hamilton Robotics, Reno, NV*
- MP 397 **LC-MS/MS Method for the Determination of 25-hydroxyvitamin D2/D3 from Serum Sample using CleanertSLE;** Suzi Qin¹; Qun Wang¹; Wan Wang¹; Warren Chen¹; ¹*Bonna Agela Technologies, Tianjin, China*
- MP 398 **LC-MS Analysis of Reserpine Using High pH Buffer ;** Subhra Bhattacharya¹; Stephen C Roemer²; ¹*Thermo Fisher Scientific, Fair Lawn, NJ*; ²*Thermo Fisher Scientific, Fair Lawn, NJ*



- MP 399 **Comparison of Three Sample Preparation Methods for Determining Perfluoroalkyl Substances, Feminizing Compounds, and Mycotoxins in Serum Using UPLC-MS/MS;** Yen-Chun Liu¹; Shin-Hung Liu¹; I-Jen Wang²; Pau-Chung Chen^{3,4}; Chia-Yang Chen^{1,4}; ¹*Institute of Environmental Health, National Taiwan University, Taipei City, Taiwan*; ²*Department of Pediatrics, Taipei Hospital, Ministry of Health and Welfare, New Taipei City, Taiwan*; ³*Institute of Occupational Medicine and Industrial Hygiene, National Taiwan University, Taipei City, Taiwan*; ⁴*Department of Public Health, National Taiwan University, Taipei City, Taiwan*
- MP 400 **Operational Impact on the Correlation of Bioanalytical Results Generated by Dried Blood Spot and Whole Blood Lysate Sampling;** Shenita Basdeo¹; Qin Ji²; ¹*Lawrenceville, NJ*; ²*BMS, Princeton, NJ*
- MP 401 **A Recombinant Asp-Specific Protease for Bottom-up Mass Spectrometry Workflows;** Chris Hosfield¹; James Hartnett¹; Alba Katiria González Rivera^{1,2}; Ethan Strauss¹; Sergei Saveliev¹; Michael Rosenblatt¹; Marjeta Urh¹; ¹*Promega Corporation, Madison, WI*; ²*University of Wisconsin Madison, Madison, WI*
- MP 402 **A Novel Strategy for the In-Process Stabilization of N-Oxide Metabolites in Hemolyzed Plasma Determined by LC-MS/MS;** Richard Lavalley¹; Georges Koudssi¹; Milton Furtado¹; Anahita Keyhani¹; ¹*Altasciences, Laval, QC, Canada*
- MP 403 **Comparison of Commonly used Anti-adsorptive Agents to Identify an Optimal Strategy to Minimize Non-specific Binding in CSF Collection;** Adam Amaral¹; Stanley I. Goldstein¹; Michael T. Rooney¹; ¹*Biogen, Cambridge, MA*
- MP 404 **Analysis of Free and Encapsulated Doxorubicin by LC-MS/MS;** Roger Demers¹; Ying Ren²; Daria L. Wentzel²; ¹*Tandem Labs, West Trenton, NJ*; ²*Covance, West Trenton, NJ*
- MP 405 **Polymeric vs Diatomaceous Earth SLE Sorbents: A Comparison of Phospholipid Depletion, Matrix Effect and Recovery for Cortisol and 6 β -Hydroxycortisol;** Laurence Mayrand Provencher¹; Sylvain Latour¹; Jeff Plomley¹; Milton Furtado¹; Anahita Keyhani¹; ¹*Altasciences, Laval, QC, Canada*
- LIPIDS: PROFILE ANALYSIS I**
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- MP 406 **Phospholipid Characterization by a TQ-MS Data Based Identification Scheme;** Tsuyoshi Nakanishi¹; Masaki Yamada¹; Ningombam Sanjib Meitei^{2,3}; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*PREMIER Biosoft, Palo Alto, CA*; ³*PREMIER Biosoft, Indore, India*
- MP 407 **Using MALDI-Mass Spectrometry Imaging to Assess the Oxidative Damage to Lipids Induced by *in vivo* Hydroxyl Radical-Based Protein Footprinting;** Jessica A. Espino¹; Claire L. Carter¹; Maureen A. Kane¹; Lisa M. Jones¹; ¹*University of Maryland School of Pharmacy, Baltimore, MD*
- MP 408 **Characterization of Cardiolipin and Monolysocardiolipin Acyl-Lipid Species in an Acute Myeloid Leukemia Cell Line;** Juan J. Aristizabal Henao¹; Ayesha K. Seneviratne²; Richard W. Smith¹; Aaron D. Schimmer²; Ken D. Stark¹; ¹*University of Waterloo, Waterloo, Ontario*; ²*Princess Margaret Cancer Centre, Toronto, ON, Canada*
- MP 409 **Comparative Analysis of Plasma Lipid Alterations Associated with Age and Dietary Restriction using Targeted MS and Untargeted LC-MS Lipidomics Approaches;** Kevin Contrepoint¹; Salah Mahmoudi¹; Anne Brunet¹; Michael Snyder¹; ¹*Stanford University, Stanford, CA*
- MP 410 **Comparative Lipidomic Profiling of Four Shellfishes by UPLC-HRMS;** Jie Xu^{1,2}; Yu Song³; Peixu Cong³; Changhu Xue³; ¹*Ocean University of China, Qingdao, China*; ²*currently as a visiting professor at the School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*; ³*College of Food Science and Engineering, Ocean University of China, Qingdao, China*
- MP 411 **An Integrated Strategy for Ganglioside Lipidomics utilizing HRMS and Skyline Software;** Asoka Ranasinghe¹; Eugene Ciccimaro²; Celia D'Arienzo²; Serhiy Hnatyshyn³; Timothy Olah²; ¹*Bristol-Myers Squibb Company, Princeton, NJ*; ²*Bristol-Myers Squibb, Princeton, New Jersey*; ³*Bristol-Myers Squibb, Princeton, NJ*
- MP 412 **LC-MSE-driven Discovery of Biomarkers for Identifying Heightened Risk of Developing Atherosclerotic Disease;** Zifeng Song¹; Gerd Bobe^{1,2}; Sahar Taqui³; Jan F. Stevens^{1,2}; Johathan Lindner³; Claudia S. Maier^{1,2}; ¹*Oregon State University, Corvallis, OR*; ²*Linus Pauling Institute, Oregon State University, Corvallis, OR*; ³*Oregon Health & Science University, Portland, OR*
- MP 413 **Analyses of Lipid Hydroperoxides in HDL and LDL of Human using Orbitrap Mass Spectrometer;** Shu-Ping Hui¹; Hitoshi Chiba¹; ¹*Faculty of Health Sciences, Hokkaido University, Sapporo, Japan*
- MP 414 **Lipidomic Studies of Beta-2-Adrenergic Receptor Agonist-induced Hepatic Steatosis in Mice;** Xiaoli Gao¹; Yun Shi¹; Dana M. Molleur¹; Susan T. Weintraub¹; Amrita Kamat¹; ¹*UT Health San Antonio, San Antonio, TX*
- MP 415 **Differential Ion Mobility Coupled to a Multi-emitter Nanoelectrospray Ion Source for Improved Shotgun Lipidomics Applications;** James E. Keating¹; Gary L. Glish¹; ¹*University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC*
- MP 416 **Pilot Study of the Plasma Lipid Profile in Ebola Vaccinated Healthy Donors using Untargeted Lipidomics Approach;** Manoj Khadka; *Emory University School of Medicine, Atlanta, GA*
- MP 417 **Mass Spectrometry-Based Characterization of Milk Lipids Isolated from Murrah Buffalo;** Kiran Ambatipudi¹; Aparna Verma¹; Sivaramaiah Nallapeta²; ¹*Indian Institute of Technology Roorkee, Roorkee, UK*; ²*Bruker Daltonics India, Centre of Excellence, Bangalore, India*
- MP 418 **Automated Lipid Profiling of Malaria Samples Using Orbitrap Velos Pro Mass Spectrometer with LipidSearch and SimLipid Software;** Ningombam Sanjib Meitei^{1,2}; Arun Apte³; Fatima Rahlouni⁴; David J. Sullivan⁵; Vladimir Shulaev⁴; ¹*PREMIER Biosoft, Palo Alto, CA*; ²*PREMIER Biosoft, Indore, India*; ³*PREMIER Biosoft, Indore, India*; ⁴*University of North Texas, Denton, TX*; ⁵*Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD*
- MP 419 **Investigating Current Limitations and Pitfalls in Lipidomics using the SRM 2378 series and Bovine Liver: A NIST Interlaboratory Study;** Candice Z. Ulmer¹; John A. Bowden¹; Christina Jones¹; Alan Heckert²; Jeremy Koelmel³; ¹*National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC*; ²*National Institute of Standards & Technology, NIST, Gaithersburg, MD*; ³*University of Florida, Department of Chemistry, Gainesville, FL*
- MP 420 **Lipid Metabolic Alterations Hallmark Pathological Processes in Human Lungs;** Lars F. Eggers¹; Julia Müller²; Chakravarthy Marella¹; Verena Scholz¹; Henrik Watz^{3,4}; Christian Kugler⁵; Klaus F. Rabe^{4,5}; Torsten Goldmann^{2,4}; Dominik Schwudke^{1,4}; ¹*Research Center Borstel, Division of Bioanalytical Chemistry, Borstel, Germany*; ²*Pathology of the University Hospital of Lübeck and the Research Center Borstel, Lübeck and Borstel, Germany*; ³*Pulmonary Research Institute at LungenClinic Großhansdorf, Großhansdorf, Germany*; ⁴*Airway Research Center North, German Center for Lung Research, Großhansdorf, Germany*; ⁵*LungenClinic Großhansdorf, Großhansdorf, Germany*
- MP 421 **Sample-per-second Shotgun Lipidomics using Acoustically-induced Electrospray Ionisation;** Martin Bachman¹; Ian Sinclair¹; Jonathan Wingfield²; Kerry



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- Hallbrook¹; Sonia Houghton¹; ¹AstraZeneca R&D, Alderley Park, UK; ²AstraZeneca R&D, Cambridge, UK
- MP 422 **MRM Based Phospholipid Profiling of Mouse Tissues by an Ultra-Fast Triple Quadrupole Mass Spectrometer;** Masaki Yamada¹; Tsuyoshi Nakanishi²; ¹Shimadzu Corporation, Kyoto; ²Shimadzu Corporation, Nakagyo-ku, Japan
- MP 423 **Robust and High Throughput Lipid Profiling in Dried Blood Spot Samples Using Automated FIA MSMS/MS Technique;** Kuldeep Ravivanshi¹; Narinder Sahni²; Akanksha Singh³; Dipanakar Malakar³; Manoj Pillai³; ¹Lipomic Healthcare Pvt. Ltd, New Delhi, India; ²Jawaharlal Nehru University, New Delhi, India; ³SCIEX, Gurugram, India
- MP 424 **Phospholipid Ratios in Drosophila and the Effects on the Reintroduction of SWS/NTE Mutations Back into Neurons using UPLC-HRMS/MS and SWATH;** Jeffrey Morre¹; Claudia S. Maier²; Brookelyn Long²; Elizabeth Sunderhaus³; Doris Kretzschmar³; ¹Oregon State University, Corvallis, OR; ²Oregon State University, Corvallis, OR; ³Oregon Health & Science University, Portland, OR
- MP 425 **Increase Sensitivity and Selectivity for Quantification of Phospholipids Based on Phosphate Methylation and MRM-based LC-MS/MS in Only Positive Ionization Mode;** Lili Niu¹; Tanxi Cai¹; Qingbo Shu¹; Xiaojing Guo¹; Xiang Ding¹; Zhensheng Xie¹; Fuquan Yang¹; ¹Institute of Biophysics, CAS, Beijing, China
- MP 426 **Development of a Rapid Method for Quantification of Branched Chain Fatty Acids in Phospholipids using Ion-Mobility Q-TOF Mass Spectrometry;** Peter S. Backlund¹; Glen W. Humphrey²; Paul S. Blank²; Alfred L. Yergey¹; Joshua Zimmerberg²; ¹NICHD, NIH, Bethesda, MD; ²Section on Membrane & Cellular Biophysics, NICHD, NIH, Bethesda, MD
- MP 427 **Lipidomic Investigation of Fenclozic Acid and Sitaxentan Treated PXB-mice using a New Scanning Quadrupole UPLC-QToF MS Acquisition Mode;** Adam King¹; Matthew Baginski²; Yoshio Morikawa²; Robert S Plumb¹; Ian D Wilson¹; ¹Imperial College, London, UK; ²PhoenixBio USA Corp., New York, NY
- MP 428 **Untargeted RP-UPLC-QTOF- MS/MS based Shotgun Lipidomics Reveals Lipid Dynamics during High Carbohydrate or High Polyunsaturated Fatty Acid Diet;** Thekkelnaycke Rajendiran¹; Tanu Soni²; Heidi Brigitte IglayReger²; Amy E Rothberg²; Charles F Burant²; ¹Dept. of Pathology, University Of Michigan, Ann Arbor, MI; ²University of Michigan Medical Center, Ann Arbor, MI
- MP 429 **Systems Biology Approach to Define the Molecular Mechanisms of Galactic Cosmic Ray induced Hepatocellular Carcinoma;** Brooke L. Barnette¹; Shinji K. Strain¹; Cheryl F. Lichti¹; Yu Yongjia¹; Robert L. Ullrich¹; Mark R. Emmett²; ¹University of Texas Medical Branch, Galveston, TX; ²University of Texas Medical Branch, Galveston, TX
- MP 430 **Analysis of Lipids Extracted from Plant and Insect Tissues using a Chromatography Based HRMS Method with Automated Data Processing ;** Daniel Gachotte¹; Yelena Adelfinskaya²; Jeffrey R Gilbert²; Jesse L Balcer²; David A Peake³; Lyudmila LV Sidorenko²; ¹Dow AgroSciences, Indianapolis, IN; ²Dow AgroSciences, Indianapolis, IN; ³ThermoFisher, San Jose, CA
- MP 431 **Lipid Profiling of Six Breast Cancer Cell Lines to Understand the Mechanism of Brain Metastatic Breast Cancer;** Masoud Zabet Moghaddam¹; Ruchika Bhawal¹; Wenjing Peng¹; Susan San Francisco¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX

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- MP 432 **Infrared Ion Spectroscopy Applied in Metabolomics and Drug Metabolism;** Jonathan Martens¹; Giel Berden¹; Rianne E. van Outersterp¹; Leo A. J. Kluijtmans²; Udo F. Engelke²; Clara D. M. van Karnebeek^{3,4}; Ron A. Wevers²; Valerie Koppen⁵; Filip Cuyckens⁵; Jos Oomens^{1,6}; ¹FELIX Laboratory - Radboud University, Nijmegen, Netherlands; ²Translational Metabolic Laboratory - Radboud University Medical Center, Nijmegen, Netherlands; ³Department of Pediatrics - University of British Columbia, Vancouver, BC, Canada, Canada; ⁴Centre for Molecular Medicine - University of British Columbia, Vancouver, BC, Canada; ⁵Pharmacokinetics, Dynamics & Metabolism - Janssen R&D, Beerse, Belgium; ⁶van't Hoff Institute for Molecular Sciences - University of Amsterdam, Amsterdam, Netherlands
- MP 433 **Merging Targeted and Non-Targeted Metabolomics via Anion-Exchange Chromatography Coupled to High Resolution Mass Spectrometry;** Michaela Schwaiger¹; Yasin El Abiead¹; Evelyn Rampler¹; Gerrit Hermann^{1,2}; Gunda Koellensperger¹; ¹University of Vienna, Vienna, Austria; ²ISOTOPIC Solutions, Vienna, Austria
- MP 434 **Redox State Alteration at the Onset of Development in D. melanogaster;** Boryana Petrova¹; Maiko Kitaoka²; Elizaveta Freinkman¹; Iva Kronja¹; Terry Orr-Weaver^{1,2}; ¹Whitehead Institute, Cambridge, MA; ²Dept. of Biology, Massachusetts Institute of Technology, Cambridge, MA
- MP 435 **Smart Data Dependent MS/MS: Toward Comprehensive MS/MS Feature Coverage in Non-Targeted Metabolomics;** Corey D Broeckling¹; Emmy Hoyes²; Jeff Brown²; Jessica E. Prenni¹; ¹Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; ²Waters Corporation, Wilmslow, UK
- MP 436 **Development of an Efficient Quantitative Assay for All Mevalonate Pathway Metabolites using Targeted LC-MS to Study Ovarian Cancer Metabolism;** Hamid R Baniasadi¹; Aaron R. Goldman¹; Hsin-Yao Tang¹; David W Speicher¹; ¹Wistar Institute, Philadelphia, PA
- MP 437 **Construction of Novel Calibration-Curve-Locking Database for Metabolomic Analysis by GC/MS;** Yuki Soma¹; Toshiyuki Yamashita¹; Kosuke Hata¹; Masatomo Takahashi¹; Kuniyo Sugitate²; Takeshi Serino²; Hiromi Miyagawa³; Kenichi Suzuki³; Takatomo Kawamukai⁴; Teruhisa Shiota⁴; Kayoko Yamada⁴; Yoshihiro Izumi¹; Takeshi Bamba¹; ¹Kyushu University, Fukuoka, Japan; ²Agilent Technologies Co. Ltd, Hachioji, Japan; ³GL Sciences Inc., Shinjuku-ku, Japan; ⁴AMR Inc., Meguro-ku, Japan
- MP 438 **Comprehensive Amino Acid and DBS Analysis with a Microchip Capillary Electrophoresis-ESI Miniature Mass Spectrometry Platform in 150 Seconds;** Michael Goodwin¹; J. Scott Mellors¹; Erin A. Redman¹; Glenn A. Harris¹; Christopher Brown¹; ¹908 Devices Inc., Boston, MA
- MP 439 **Challenging the C1 Folate Cycle Paradigm with Probiotic Lactobacillus reuteri;** Abby J Chiang¹; Daniel Röth¹; Gabriel Gugiu¹; James Versalovic²; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Texas Children's Hospital, Houston, TX
- MP 440 **Direct Analysis of Terpenes from Biologically Relevant Buffers using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI);** Milad Nazari¹; Sean R. Lund¹; Gavin J. Williams¹; Jon D. Williams²; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²AbbVie, North Chicago, IL
- MP 441 **Metabolomics of Biofluids from Nonhuman Primate Exposed to Ionizing Radiation;** Evan Pannkuk¹; Evagelia C Laiakis²; Simon Authier³; Karen Wong³; Albert J. Fornace^{1,2}; ¹Tumor Biology Program, Lombardi Comprehensive



- Cancer Center, Georgetown University, Washington, DC;
²Department of Biochemistry and Molecular & Cellular Biology, Georgetown University, Washington, DC;
³CiToxLAB North America, Laval, QC, Canada
- MP 442 **Integration of Volumetric Absorptive Microsampling with a Mass Spectrometry-Based Metabolomics Workflow;** Giuseppe Paglia¹; Chiara Volani^{1,2}; Giulia Caprioli¹; Baldur Sigurdsson¹; Guenter Weiss²; Sigurdur Smarason¹; ¹EURAC Research, Bolzano, Italy; ²Medical University of Innsbruck, Innsbruck, Austria
- MP 443 **Metabolomics of Cotton Fiber;** Manoj S. Ghaste¹; Vladimir Shulaev¹; ¹Department of Biological Sciences, University of North Texas, Denton, TX
- MP 444 **Combining Benzoyl Chloride Derivatization with Accurate Mass Qualitative and Quantitative Analysis to Increase Understanding of Neurological Systems;** Stefan Thibodeaux¹; Kimberly Malesky¹; Madeline Weber¹; Clayton Springer¹; Shu Li¹; ¹Novartis, Cambridge, MA
- MP 445 **Analysis of Non-Mevalonate (MEP) Pathway Standards and Metabolites in Cell Lysate Using a Novel LC-MS/MS Method;** Allison Fabino Carr¹; Michael Lesslie¹; Darshan C. Patel²; Victor V. Ryzhov¹; Daniel W. Armstrong²; ¹Northern Illinois University, DeKalb, IL; ²University of Texas at Arlington, Arlington, TX
- MP 446 **Evaluation of Different Cell Harvesting and Lysis Methods for Chemical Isotope Labeling LC-MS Metabolomics;** Xinyun Gu¹; Xian Luo¹; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada
- MP 447 **Metabolic Changes in Lung Tissue of Tuberculosis-Infected Mice using GC/Q-TOF;** ^{M^a} Fernanda Rey-Stolle¹; Vineel P Reddy²; Santiago Angulo¹; Adrie JC Steyn^{2,3,4}; Sofia Nieto⁵; Nathan Eno⁵; Coral Barbas¹; ¹CEMBIO (Centro de Metabolómica y Bioanálisis), Facultad de Farmacia, Universidad CEU San Pablo, Madrid, Spain; ²Department of Microbiology, University of Alabama at Birmingham, Birmingham, AL; ³KRITH (KwaZulu-Natal Research Institute for TB and HIV), Durban, South Africa; ⁴UAB Center for Free Radical Biology, University of Alabama at Birmingham, Birmingham, AL; ⁵Agilent Technologies Inc., Santa Clara, CA
- MP 448 **Metabolomic Approach for Carotenoids Analysis of Chrysanthemum Flower by Liquid Chromatograph Tandem Mass Spectrometry;** Junichi Masuda¹; Satoshi Yamaki²; Yoshihiro Hayakawa²; Masaru Furuta²; Yuji Sawada³; Mami Okamoto³; Muneo Sato³; Masami Y. Hirai³; ¹Shimadzu Corporation, Hadano-city, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa
- MP 449 **Quantitative and Qualitative Metabolic Flux Analysis via a Novel Data Independent Acquisition Mode 'SONAR' using High Resolution Mass Spectrometry;** Paul Rainville¹; Chris Beecher²; Jose Castro-Perez³; James Langridge⁴; David Heywood⁴; ¹Waters, Milford, MA; ²IROA Technologies, Gainesville, Florida; ³Waters Corp, Milford, MA; ⁴Waters Corp., Wilmslow, UK
- MP 450 **Metabolomic Analysis of Microbiome Transplantation in Mice;** Jason Winnike¹; David Kirchner¹; Kevin Knagge¹; Brian Bennett²; ¹David H. Murdock Research Institute, Kannapolis, NC; ²United States Department of Agriculture Agricultural Research Service, Davis, CA
- MP 451 **Metabolomic Interrogation of the Mechanisms of Radiation-Induced Lung Injury;** Jenna Alloush¹; Jace W. Jones²; Claire Louise Carter²; Isabel L Jackson³; Zeljko Vujaskovic³; Maureen A Kane²; ¹Baltimore, MD; ²University of Maryland School of Pharmacy, Baltimore, MD; ³University of Maryland School of Medicine, Baltimore, MD
- MP 452 **Application of Isotopically Nonstationary Flux Analysis for Nucleotides Metabolism Studies in Human Cells;** Fedor Kryuchkov; University of Bergen, Bergen, Norway
- MP 453 **Comprehensive Analysis of Hydrophilic Metabolites by Coupling Ion Chromatography and PFPP-based Liquid Chromatography Methods to High Resolution Mass Spectrometry;** Yoshihiro Izumi¹; Takahiro Suzuki²; Masatomo Takahashi¹; Kohta Nakatani¹; Kiyotaka Oshikawa¹; Motokazu Kimura²; Takahara Kentaro²; Masaki Matsumoto¹; Takeshi Bamba¹; ¹Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; ²Thermo Fisher Scientific Japan, Tokyo, Japan
- MP 454 **Targeted LC-MS/MS Based Metabolomics Revealing Staphylococcus aureus Metabolic Reprograming, from Planktonic to Biofilm;** Chen Wang¹; Jiangjiang Zhu¹; ¹Miami University, Oxford, Ohio
- MP 455 **Mice Fecal Metabolomics by LC-MS/MS: Comparison between Young Mice and Old Mice;** Takanari Hattori^{1,2}; Shuichi Kawana¹; Yoshihiro Hayakawa¹; Eiichihiro Fukusaki³; Mitsuharu Matsumoto⁴; ¹Shimadzu Corporation, Kyoto, Japan; ²Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan; ³Osaka University, Suita, Japan; ⁴Kyodo Milk Industry Co. Ltd., Nishitama, Japan
- MP 456 **Steroid and Tricarboxylic Acid Cycle Isobar Separation and Quantitation using Ion Mobility-QTOF and LC/MS/MS;** Sumankalai Ramachandran¹; Minas Sakellakis¹; Zahi Mitri²; Niki Millward³; Sriram Shanmuga Velandy³; Pratip Bhattacharya³; David Piwnicka-Worms³; Christopher Logothetis¹; Mark Titus¹; ¹Koch Center, MD Anderson Cancer Center, Houston, TX; ²Oregon Health & Science University, Portland, OR; ³Cancer Systems Imaging, MD Anderson Cancer Center, Houston, TX
- MP 457 **High-throughput Analysis of Xenobiotics by Automated Electrochemistry/Mass Spectrometry;** Simon Gereon Scheeren¹; Uwe Karst¹; ¹University of Münster, Institute of Inorganic and Analytical Chemistry, Münster
- MP 458 **Targeted and Untargeted Mass Spectrometry for Identification of Metabolomic Changes Associated with Chronic Defeat Stress in Mice;** Constance A. Sobsey¹; Jun Han¹; Michael J. Meaney^{2,3,4}; Christoph H. Borchers^{1,3,5}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada; ³Dept. of Oncology, McGill University, Montreal, QC, Canada; ⁴Depts. of Psychiatry and Neurology and Neurosurgery, McGill University, Montreal, QC, Canada; ⁵Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 459 **Development of More Reproducible and Sensitive Polar Metabolomics Methods;** Hardik Shah¹; Steven M. Fischer²; Justin R. Cross¹; ¹Donald B. and Catherine C. Marron Cancer Metabolism Center at Memorial Sloan Kettering Cancer Center, New York, NY; ²Agilent Technologies, Santa Clara, CA
- MP 460 **Same Sample Targeted and Untargeted Fecal Mass Spectrometry for Molecule - Microbiome Wide Association Studies;** Alexey V. Melnik¹; Ricardo Da Silva¹; Embriette R Hyde²; Fernando Vargas¹; Amina Bouslimani¹; Ivan Protsyuk³; Alan Jarmusch¹; Alexander Aksenov¹; Anupriya Tripathi^{1,2,4}; Theodore Alexandrov^{1,3,5}; Rob Knight^{2,4}; Pieter C. Dorrestein^{1,2}; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ²Department of Pediatrics, University of California San Diego, La Jolla, CA; ³EMBL, Heidelberg, Heidelberg; ⁴Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; ⁵Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA
- MP 461 **Identification of Metabolite Markers of Mn2+ Accumulation in Deinococcus radiodurans by Liquid Chromatography Mass Spectrometry;** Jingyueh Jeng; Chia Nan Univ of Pharmacy & Science, Tainan, Asia



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- MP 462 **Semi-targeted Metabolomics of Oxylipins**; Jeffrey F. Kuhn¹; Fred Bjorn Lih¹; Matthew Edin¹; Darryl Zeldin¹; Leesa J Deterding¹; ¹NIEHS/NIH/DHHS, Research Triangle Park, NC
- MP 463 **LC-MS Metabolomic Serum Signatures Indicate Changes in Protein and Fatty Acid Metabolism Precede Retained Placenta in Dairy Cows**; Fereshteh Zandkarimi¹; Gerd Bobe^{2,3}; Claudia S. Maier^{1,3}; ¹Chemistry Department, Oregon State University, Corvallis, OR; ²Department of Animal and Rangeland Sciences, Corvallis, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR

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- MP 464 **Coupling Solid Phase Microextraction to Complementary Separation Platforms for Metabotyping of E. coli Metabolome in Response to Natural Antibacterial Agents**; Fatemeh Mousavi¹; Emanuela Gionfriddo²; Eduardo Carasek³; Erica A Souza-Silva⁴; Janusz Pawliszyn²; ¹Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON, Canada; ²University of Waterloo, Waterloo, Ontario; ³Department of Chemistry, Federal University of Santa Catarina, Florianópolis, Brazil; ⁴Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil
- MP 465 **An Approach for Metabolomics Survey of the Extracellular Vesicles in Esophageal Carcinoma Serum**; Yan Ren¹; Ju Wang¹; Jin Zi¹; Liang Lin¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China
- MP 466 **Automated Sample Preparation for GC/MS and LC/MS-based Metabolomics: Analysis of Contamination Sources**; Emily Davidson¹; Sarah-Marie A Lyons¹; Corey D. Broeckling¹; Jessica E. Prenni¹; ¹Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO
- MP 467 **A LC-MS Metabolomics Method Enabling Rapid Sample Preparation and Analysis of Polar and Unstable Metabolic Intermediates**; Tony Karlsborn¹; Magesh Muthu¹; Anders Nordström¹; ¹Department of Molecular Biology, Umeå University, Umeå, Sweden
- MP 468 **Assessment of Rapid Heat Treatment for Pre-Analytical Stabilization of the Lipidome**; Christina M Jones¹; Jeremy P Koelmel²; Tracey B Schock¹; Candice Z. Ulmer¹; John A. Bowden¹; ¹National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; ²University of Florida, Department of Chemistry, Gainesville, FL
- MP 469 **Method Development for the Metabolomic Profile of Cyanobacteria with Altered Circadian Rhythms**; Berkley Ellis¹; R. L. Gant-Branum²; Chi Zao³; Yao Zu³; Carl H Johnson²; John A. McLean²; ¹, Nashville, TN; ²Vanderbilt University, Nashville, TN; ³Vanderbilt University, Nashville, TN
- MP 470 **Untargeted Metabolomic and Lipidomic Characterization of Brain Tissue using Solid Phase Microextraction**; Ezel Boyaci¹; Nathaly Reyes-Garcés¹; German A Gómez-Ríos¹; Barbara Bojko^{1,2}; Dajana Vuckovic³; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON, Canada; ²Nicolaus Copernicus University in Torun, Bydgoszcz, Poland; ³Concordia University, Montreal, QC, Canada
- MP 471 **Automation of Sample Preparation Procedure for Hydrophilic Metabolomic and Lipidomic Analysis using a Robotic Platform**; Yuki Soma¹; Toshiyuki Yamashita¹; Masatomo Takahashi¹; Kuniyo Sugitate²; Takeshi Serino²; Hiromi Miyagawa³; Kenichi Suzuki³; Takatomo Kawamukai⁴; Teruhisa Shiota⁴; Kayoko Yamada⁴; Yoshihiro Izumi¹; Takeshi Bamba¹; ¹Kyushu University, Fukuoka, Japan; ²Agilent Technologies Co. Ltd, Hachioji, Japan; ³GL Sciences Inc., Shinjuku-ku, Japan; ⁴AMR Inc., Meguro-ku, Japan

- MP 472 **Improving Metabolite Extraction in Metabolomics with Crosslinkers**; Kevin Y Cho¹; Liz Llufrío¹; Xiangfeng Niu¹; Gary J. Patti¹; ¹Washington University School of Medicine, St. Louis, MO
- MP 473 **Extraction and Quantitation of NAD(P)(H)**; Wenyun Lu¹; Li Chen¹; Sheng Hui¹; Joshua D Rabinowitz¹; ¹Princeton University, Princeton, NJ
- MP 474 **Evaluation of an Automated LC-MS/MS System for Analyzing Hydrophilic Blood Metabolites**; Shin Nishiumi¹; Keisuke Shima²; Hidekazu Saiki²; Takeshi Azuma¹; Masaru Yoshida^{1,3}; ¹Kobe University Graduate School of Medicine, Kobe, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³AMED, Kobe, Japan

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS I 475 - 495

- MP 475 **Liquid Chromatography Tandem Mass Spectrometric Analysis of Bile Acids in Biological Samples**; Jaeman Byun¹; Anna V. Mathew¹; Adil Jadoon¹; Subramaniam Pennathur¹; ¹University of Michigan, Ann Arbor, MI
- MP 476 **N-omics: Metabolomics for N-containing Metabolites**; Ryo Nakabayashi¹; Kei Hashimoto¹; Tetsuya Mori¹; Kiminori Toyooka¹; Kazuki Saito^{1,2}; ¹RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa; ²Chiba University, Chiba, Japan
- MP 477 **Multivariate Approach to Optimize a Novel Diagnostic One-Pot Derivatization Kit for Biomarkers of BTEX**; Yehia Baghdady¹; Kevin A. Schug¹; ¹The University of Texas at Arlington, Arlington, TX
- MP 478 **Identification and Quantitation of Long Chain Fatty Acids by Targeted Metabolomics**; Chandra Shekar R Ambati¹; Nagireddy Putluri¹; Arun Sreekumar¹; Vivekananda Shetty¹; ¹Baylor College of Medicine, Houston, TX
- MP 479 **Human Plasma Targeted-Metabolomics Using an Amine Derivatization Reagent**; Kazutaka Shimbo; Ajinomoto CO., INC, Kawasaki-Shi, Kanagawa
- MP 480 **Using Metabolomics to Characterize Marine Organic Matter Cycling by Microbes**; Melissa C. Kido Soule¹; Krista Longnecker¹; Cara L. Fiore²; Jamie W. Becker³; Rogier Braakman³; Keven Dooley³; Allison Coe³; Sallie W. Chisholm³; Elizabeth B. Kujawinski¹; ¹Woods Hole Oceanographic Ins, Woods Hole, MA; ²Appalachian State University, Boone, North Carolina; ³Massachusetts Institute of Technology, Cambridge, MA
- MP 481 **An Isotope-Labeling Chemical Derivatization - UPLC/MS/MS Method for Accurate Quantitation and Stability Testing of Carnitines in Dried Blood Spots**; Jun Han¹; Rehan Higgins¹; Juncong Yang¹; Karen Lin¹; Kieran Atkinson¹; Christoph H. Borchers^{1,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 482 **A Targeted LC-MS/MS Method for Separation and Quantification of Numerous Vitamin D Metabolites including 1 α ,25(OH) $_2$ D, 3-EPI-25OHD3, and 25OHD3**; Brian C Defelice^{1,2}; Oliver Fiehn^{1,2}; ¹West Coast Metabolomics Center, Davis, CA; ²University of California, Davis, Davis, CA
- MP 483 **Collaborative Cross Founder Mouse Strain Profiling via Targeted Metabolomic Library**; Dorothy Ahlf Wheatcraft¹; Rob Wilpan²; Ruth Saxl²; ¹Jackson Laboratory, Bar Harbor, ME; ²The Jackson Laboratory, Bar Harbor, ME
- MP 484 **Evaluation of High Speed, High Resolution Data Independent Acquisition for Simultaneous Identification and Quantitative Metabolomic Flux Analysis**; Loren Olson¹; Emile Plise²; Baljit Ubhi¹; ¹SCIEX, Redwood City, CA; ²Genentech, Inc, South San Francisco, CA



- MP 485 **Validation and Characterization of the iROA Standard Library using High Resolution Mass Spectrometry;** Vilinh Tran¹; Ken Liu¹; Dean P Jones¹; ¹Emory School of Medicine, Atlanta, GA
- MP 486 **Detection and Quantitation of Sugar Phosphate Metabolite Markers in Femto Molar Concentration using 6500+ QTRAP LCMS/MS System;** Manoj Pillai¹; Dipankar Malakar¹; Faraz Rashid¹; ¹ABSCIEX, Gurgaon, Haryana
- MP 487 **Separation, Identification and Quantification of Peptidoglycan Fragments by Zwitterionic Hydrophilic Interaction Chromatography and Capillary Electrophoresis Coupled to Mass Spectrometry;** Madeleine Boulanger^{1,2}; Alice Raymackers²; Cédric Delvaux¹; Johann Far¹; Loïc Quinton¹; Edwin De Pauw¹; Bernard Joris²; ¹Mass Spectrometry Laboratory, Liège, Belgium; ²Center for Protein Engineering, Liège, Belgium
- MP 488 **Quantitative Profiling of Central Carbon Metabolites by Liquid Chromatography-Mass Spectrometry;** Yan-Ping Lin¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- MP 489 **Nano LC-MS/MS Method Development for the Analysis of Steroids in Whale Blubber for Reproductive Fitness and Stress Assessments;** Ruchika Bhawal¹; Mary Hayden¹; John Escobedo¹; Clinton Harmon¹; David Klein¹; Susan San Francisco¹; Masoud Zabet Moghaddam¹; Celine Godard-Codding¹; ¹Texas Tech University, Lubbock, TX
- MP 490 **Targeting the Long Game: Assessing Longitudinal Precision and Bias of Two Targeted Metabolomics Platforms in the Context of Clinical Metabolomics;** J. Will Thompson¹; Lisa St. John-Williams¹; M. Arthur Moseley¹; ¹Duke University School of Medicine, Durham, NC
- MP 491 **Quantification of Amino Acids using Isotopic Ratio Outlier Analysis (IROA) and LC-MS/MS;** Vanessa Y. Rubio¹; Chris Beecher^{2,3}; Richard A. Yost¹; Timothy J. Garrett⁴; ¹University of Florida, Department of Chemistry, Gainesville, FL; ²IROA Technologies, Gainesville, Florida; ³University of Florida, Gainesville, FL; ⁴University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL
- MP 492 **Quantitative LC-MS/MS Analysis of 100 Intracellular Metabolites of Clostridium autoethanogenum using Multiple Uniformly 13C-labelled Internal Standards;** Laudina Safo¹; Alex Grosse-Honebrink²; Salah Abdelrazig²; Bart Pander²; Anne M. Henstra²; Rupert Norman²; Thomas Millat²; Neil R Thomas²; Klaus Winzer²; Dong-Hyun kim²; Nigel Minton²; David A. Barrett²; ¹University of Nottingham, Nottingham, UK; ²University of Nottingham, School of Pharmacy, Nottingham, UK
- MP 493 **Determination of TCA Metabolites by Ion Chromatography HR/AM Mass Spectrometry;** Terri T. Christison¹; Shen Hu²; Ralf Tautenhahn¹; Reiko Kiyonami¹; Jeffrey S Rohrer¹; ¹Thermo Fisher Scientific, San Jose, CA; ²University of California, Los Angeles, Los Angeles, CA
- MP 494 **Targeted Metabolomics using LC-QqQLIT, Data-Dependent Acquisition, and Scheduled SRM;** Michel Wagner¹; Marc Turgeon¹; George Poulogiannis¹; ¹The Institute of Cancer Research, London
- MP 495 **Solvent-compensation liquid Chromatography System Coupled with Multiple Detectors in the Analysis of Metabolites Related to the Quality of Tea;** Che-I Liao¹; Zong-Yi Wu¹; Kuo-Lung Ku¹; ¹National Chiayi University, Chiayi City, Taiwan
- METABOLOMICS: UNTARGETED METABOLITE PROFILING I**
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- MP 496 **Comparative Metabolic Profiling of Metastatic and Primary Melanoma Cell Lines;** Zhihao Yu¹; Ming Huang²; Brian Clowers¹; ¹Washington State University, Pullman, WA; ²University of California, Riverside, Riverside, CA
- MP 497 **Separating Metabolites Basing on Their Structural Properties: A Metabolomics Case Study, and Potential Path to Molecular Structure Digitization;** Gang Xing¹; Michelle F. Clasquin¹; Meihua Tu¹; Thomas V. Magee¹; ¹Pfizer, Cambridge, MA
- MP 498 **Molecular Biogeography of the Heart Identifies Determinants of Chagas Disease Progression;** Laura-Isobel McCall¹; James T. Morton¹; Jair Lage de Siqueira-Neto¹; Rob Knight¹; Pieter C. Dorrestein¹; James H. McKerrrow¹; ¹University of California San Diego, San Diego, CA
- MP 499 **Multiplatform Metabolomics Reveals Predictive Prostate Cancer Recurrence Phenotypes Following Radical Prostatectomy;** Chaevien S. Clendinen¹; David A. Gaul¹; Rebecca S. Arnold²; Arthur S. Edison³; John A. Petros^{2,4}; ¹Georgia Institute of Technology, Atlanta, GA; ²Emory University, Atlanta, Georgia; ³University of Georgia, Athens, GA; ⁴Atlanta VA Medical Center, Atlanta, GA
- MP 500 **Metabolomic Signatures in Urine from Renal Cell Carcinoma Patients;** David A. Gaul¹; Chaevien S. Clendinen¹; Rebecca S. Arnold²; John A. Petros²; Facundo M. Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Emory University, Atlanta, GA
- MP 501 **Proteomics and Metabolomics Profiles of Endothelial Cells under High and low Shear Stress: Understanding the Atherosclerosis Onset at Molecular Level;** Gabriela Venturini Silva¹; Rafael Dariolli¹; Kallyandra Padilha¹; Pamella Araujo Malagrino¹; Tamiris Gois¹; Valdemir Melechco Carvalho²; Jessica Silva Salgueiro²; Karina Moraes Cardozo²; Jose Eduardo Krieger¹; Alexandre Costa Pereira¹; ¹Incor - FMUSP, Sao Paulo, Brazil; ²Fleury Group, Sao Paulo, Brazil
- MP 502 **Curatr: A Browser Based Platform for Building High Quality Spectral Libraries;** Andrew Palmer¹; Prasad Phapale¹; Dominik Fay¹; Theodore Alexandrov^{1,2}; ¹EMBL, Heidelberg, Baden-Wuerttemberg; ²Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA
- MP 503 **A Pilot Multiplatform Metabolomic Fingerprinting Study of Plasma Metabolic Alterations in Breast Cancer;** Mónica Cala¹; Julian Aldana¹; Jessica Medina²; Julian Sanchez³; Jose Guio³; Julien Wist²; Roland Meesters¹; ¹Universidad de los Andes, Bogotá, D.C., Colombia; ²Universidad del Valle, Cali, Colombia; ³Liga contra el Cancer Seccional Bogotá, Bogotá, D.C., Colombia
- MP 504 **Intra- and Inter-Lab LC-MS Data Comparison for Studying Portability of a Metabolite Library for Rapid Metabolite Identification in Metabolomics;** Shuang Zhao¹; Xian Luo¹; Ulrike Schweiger Hufnagel²; Aiko Barsch²; Liang Li¹; ¹University of Alberta, Edmonton, Alberta; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 505 **Metabolomic Profile of Tambaqui Fish (Colossoma macropomum, Cuvier 1818) under Hypoxia;** Clécio Fernando Klitzke¹; Marcos N. Eberlin²; Adalberto L. Val¹; ¹Laboratory of Ecophysiology and Molecular Evolution, Brazilian National Institute for Research of the Amazon, Manaus, Brazil; ²Thomson Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas, Campinas, Brazil
- MP 506 **Development of Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Profiling the Carbonyl Submetabolome;** Shuang Zhao¹; Margot Dawe¹; Kevin Guo¹; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada, Canada



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- MP 507 **Changes in Plasma Metabolites of Patients with Atrial Fibrillation;** Youngee Jung^{1,2}; Geum-Sook Hwang^{1,3}; ¹Western Seoul Center, Korea Basic Science Institute, Seoul, South Korea; ²Department of Life Science, Ewha Womans University, Seoul, South Korea; ³Department of Chemistry and Nano Science, Ewha Womans University, Seoul, South Korea
- MP 508 **Profiling of Polyphenols in Fruits and Vegetables by UPLC-(ESI)-QToF-MS with UNIFI-based Data Processing;** Dasharath Pandurang Oulkar¹; Zareen Khan¹; Kaushik Banerjee¹; ¹National Referral Laboratory, ICAR-National Research Centre for Grapes, Manjri Farm, Pune, India
- MP 509 **Determining Impacts of a Natural Product Biosynthetic Pathway on Streptomyces Metabolomes by Isotopic Ratio Outlier Analysis (IROA) Global Metabolomics;** Amy L Lane¹; Elle D James¹; Felice A de Jong²; Chris Beecher³; ¹University of North Florida, Jacksonville, FL; ²IROA Technologies LLC, Bolton, MA; ³University of Florida, Gainesville, FL
- MP 510 **MALDI-MSI Allows Identification and Semi-Quantification of Endogenous Cardenolides Associated with Glioblastoma Cells Death under ZIKV Infection;** Estela de Oliveira Lima¹; Tatiane Melina Guerreiro¹; Carlos Fernando O. R. Melo¹; Diogo Noin de Oliveira¹; Daisy Machado²; Marcelo Lancellotti²; Rodrigo Ramos Catharino¹; ¹Innovare Biomarkers Laboratory, Campinas, Brazil; ²Laboratory of Biotechnology, Campinas, Brazil
- MP 511 **Global Metabolomic Investigation of Tissues from Melanoma Patients with HRMS Using a Yeast Standard for Isotopic Ratio Outlier Analysis (IROA);** Taylor M. Domenick¹; Chris Beecher^{2,3}; Louis Searcy¹; Peter A. Kanetsky⁴; Richard A. Yost¹; Nicholas Taylor⁵; Timothy J. Garrett⁶; ¹University of Florida, Department of Chemistry, Gainesville, FL; ²IROA Technologies, Gainesville, Florida; ³University of Florida, Gainesville, FL; ⁴H. Lee Moffitt Cancer Center and Research Institute, Tampa, FL; ⁵Texas A&M University, College Station, TX; ⁶University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL
- MP 512 **Metabolomic Studies of Pyrazinamide in Mycobacterium Tuberculosis Using an Ion-pairing Reverse Phase Q-TOF LC/MS Approach;** Yugin Dai¹; Travis E Hartman²; Steve M Fischer¹; Kyu Y Rhee^{2,3}; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Division of Infectious Diseases, Department of Medicine, Weill Cornell Medical College, New York, NY; ³Department of Microbiology and Immunology, Weill Cornell Medical College, New York, NY
- MP 513 **Global Plasma Metabolic Profiles in Term and Preterm Birth;** Brittany Lee-McMullen¹; Kevin Contrepois¹; Martin Angst¹; Brice Gaudillere¹; Stephen Quake¹; David A. Relman¹; Gary M. Shaw¹; David K. Stevenson¹; Mike Snyder¹; ¹Stanford University, Stanford, CA
- MP 514 **Metabolic Effects in Atorvastatin-Treated Liver Cells;** Gabriela Venturini¹; Kallyandra Padilha¹; Rafael Dariolli¹; Pamela Araujo Malagrino¹; Jose Eduardo Krieger¹; Alexandre Costa Pereira¹; ¹Heart Institute, Sao Paulo, SP
- MP 515 **Untargeted Investigation of Non-alcoholic Fatty Liver Disease Using Effective Multiplatform GC-MS Instrumentation;** David Alonso¹; Xiang Zhang²; Joe Binkley³; ¹LECO Corporation, St. Joseph, MI; ²University of Louisville, Louisville, KY; ³LECO Corporation, St Joseph, MI
- MP 516 **The Effect of Sleep and Circadian Disruption on the Human Metabolome;** Fernando Vargas¹; Christopher Depner²; Antonio González Peña³; Kenneth Wright²; Rob Knight³; Pieter C. Dorrestein¹; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ²University of Colorado, Boulder, CO; ³Department of Pediatrics, University of California San Diego, San Diego, CA
- MP 517 **Untargeted Metabolomics Reveals Novel Metabolites within the Coastal and Open Ocean;** Elizabeth Kujawinski¹; Winifred Johnson¹; Melissa C. Kido Soule¹; Krista Longnecker¹; ¹Woods Hole Oceanographic Inst., Woods Hole, MA
- MP 518 **Utilizing an Untargeted Ion Mobility-Mass Spectrometry Method to Profile Changes in the Gut Metabolome;** James Poland¹; Alexandra C Schrimpe-Rutledge¹; Charles Robb Flynn¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- MP 519 **Metabolic Reprogramming by ETHE1, a Mitochondrial Persulfide Dioxygenase;** Changyuan Lu¹; Joshua Benjamin Zuk¹; Steven Gross¹; ¹Weill Medical College of Cornell, New York, NY

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- MP 520 **Novel Capillary Flow LC HRAM MS Platform for Fast Targeted Analysis and Robust Profiling of Complex Samples;** Alexander Boychenko¹; Martin Ruehl¹; Peter Bults²; Stephan Meding¹; Mike Baynham³; Wim Decrop¹; Alexander Harder⁴; Nico Van De Merbel²; Rainer Bischoff²; Remco Swart¹; ¹Thermo Fisher Scientific, Germering, Germany; ²University of Groningen, Groningen, Netherlands; ³Thermo Fisher Scientific, Runcorn, UK; ⁴Thermo Fisher Scientific, Bremen, Germany
- MP 521 **An HS-MRM Assay for Quantification of Host Cell Proteins in Therapeutic Monoclonal Antibodies;** Catalin Doneanu¹; Jing Fang²; Yun Alelyunas²; Ying Qing Yu²; Mark Wrona²; Weibin Chen²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Milford, MA
- MP 522 **An Open-Source Tool for the Creation of Multiplexed, Targeted Proteomic Instrument Methods Utilizing Isobaric Labels;** Christopher Rose^{1,2}; Brian K Erickson²; Steven Gygi²; Donald Kirkpatrick¹; ¹Genentech, Inc., South San Francisco, CA; ²Harvard Medical School, Boston, MA
- MP 523 **Building ProteomeTools Based on a Complete Synthetic Human Proteome;** Daniel P. Zolg¹; Mathias Wilhelm¹; Karten Schnatbaum²; Johannes Zerweck²; Tobias Knaute²; Bernard Delanghe³; Hans-Christian Ehrlich⁴; Peng Yu¹; Siegfried Gessulat^{1,4}; Maximilian Weiniger¹; Tobias K Schmidt¹; Patroklos Samaras¹; Karl Kramer¹; Judith Schlegel⁵; Holger Wenschuh²; Thomas Moehring³; Stephan Aiche⁴; Andreas F. Huhmer⁶; Ulf Reimer²; Bernhard Kuster^{1,7}; ¹Technical University of Munich, Freising, Germany; ²JPT Peptide Technologies GmbH, Berlin, Germany; ³Thermo Fisher Scientific, Bremen, Germany; ⁴SAP SE, Potsdam, Germany; ⁵SAP SE, Walldorf, Germany; ⁶ThermoFisher, San Jose, CA; ⁷Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany
- MP 524 **A Highly Effective Workflow for the Targeted Detection of Peptides in Complex Biological Sample Matrices from Discovery to Quantitation;** David Sarracino¹; Susan E Abbatiello¹; Scott Peterman¹; Amol Prakash²; Shen Luan¹; Claudia Martins³; Mary Blackburn³; ¹Thermo Scientific, Cambridge, MA; ²Optys Technologies, Boston, MA; ³Thermo Fisher Scientific, San Jose, CA
- MP 525 **Designing Targeted Detection of Peptides in Complex Matrices combining the MIDAS™ Workflow with the Skyline Software;** Jenny Albanese¹; Christie Hunter²; Kaipo Tamura³; Brendan MacLean⁴; ¹Jenny Albanese, Redwood City, CA; ²Christie L. Hunter, Redwood City, CA; ³Kaipo Tamura, Seattle, WA 98105; ⁴Brendan, Seattle, WA
- MP 526 **Optimized Peptide Retention Time Standards for Targeted Proteomics;** Lawrence Eckler¹; Karsten Schnatbaum¹; Daniel Zlog²; Tobias Knaute¹; Mathias Wilhelm³; Bernhard Kuster⁴; ¹JPT Peptide Technologies, Berlin; ²Technical University of Munich, Freising, Germany; ³Center for Integrated Protein Science Munich, Freising, Germany; ⁴Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany



- MP 527 **Proteomic Connectivity Maps of Chromatin and Phosphosignaling: Community Resources for Drug Discovery and Functional Genomics**; Lev Litichevskiy¹; Adam Officer¹; Amanda Creech¹; Shawn Egri¹; Malvina Papanastasiou¹; Ryan Peckner¹; Xiaodong Lu¹; Daniel Lam¹; Desiree Davison¹; Tak Ko²; Vagisha Sharma³; Fatema Abdurrob²; Jennie Z. Young²; David L. Lahr¹; Alison Mungenast²; Jarrett Egerton³; Steven A. Carr¹; Michael J MacCoss³; Li-Huei Tsai²; Jacob D. Jaffe¹; ¹The Broad Institute, Cambridge, MA; ²Massachusetts Institute of Technology, Cambridge, MA; ³University of Washington, Seattle, WA
- MP 528 **Scout-MRM Simplifies Targeted Assay Development from Public Proteomic Dataset: A Yeast Proteome Case Study**; Lény Garcia¹; Romain Carriere¹; Eric Testet²; Pathy Laquel³; François Doignon³; Yves LeBlanc⁴; Aycirix Sophie¹; Jérôme Lemoine⁵; ¹Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France; ²Institut Polytechnique de Bordeaux, Bordeaux, France; ³Université de Bordeaux, Bordeaux, France; ⁴SCIEX, Concord, ON, Canada, ON, Canada; ⁵Université de Lyon, Villeurbanne
- MP 529 **Towards Accurate Multiplexed Protein Mass Spectrometry for the Masses**; Martin Wühr¹; Graeme McAlister²; Matthew Sonnett¹; ¹Princeton University, Princeton, NJ; ²ThermoFisher, San Jose, CA
- MP 530 **Trends in Disulfide Bond Formation in Cysteine Containing Small Peptides**; Michael D. Browne¹; LeRoi de-Souza¹; Ekram Hossain¹; Jianhua Ren¹; ¹University of the Pacific, Stockton, CA
- MP 531 **Selective Capture and Analysis of Azido Compounds Using a Propargyl-based Cleavable Linker**; Michael G.J. Doyle¹; Baylie Gigolyk¹; Michelle McEllan¹; Vinith Yathindranath¹; Edward D Bodnar²; Helene Perreault³; ¹University of Manitoba, Winnipeg, MB; ²Agilent Technologies, Inc., Wilmington, DE; ³University of Manitoba, Winnipeg, MB
- MP 532 **Bioanalytical Method Development for Therapeutic Peptides: Strategies for Overcoming LC/MS/MS-based Assay Hurdles**; Moucun Yuan¹; Eric Ma¹; William Mylott¹; Rand Jenkins¹; ¹PPD Laboratories, Richmond, VA
- MP 533 **Targeted Neuropeptidomics: Parallel Reaction Monitoring or Data-Independent Acquisition for the Analysis of Neuropeptides using High-Resolution Mass Spectrometry**; Mouna Saidi¹; Soufiane Kamali¹; Francis Beaudry¹; ¹Université de Montréal, St-Hyacinthe, QC, Canada
- MP 534 **Implementation of Capillary Zone Electrophoresis Methods in Quantitative Proteomics**; Simon Kreimer¹; Benjamin C Orsburn²; Robert N. O'mealy¹; Robert N. Cole¹; ¹Mass Spectrometry and Proteomics Facility, Johns Hopkins School of Medicine, Baltimore, Maryland; ²Thermo Fisher Scientific, Baltimore, Maryland
- MP 535 **Using Electrokinetic Injection to Increase Throughput and Improve Sensitivity in the Detection of Basic Neuropeptides by Capillary Electrospray Ionisation (CESI)**; Stephen J. Lock¹; Jim Thorn¹; Edna Betgovarguez²; Bryan Fonslow²; ¹SCIEX, Warrington, UK; ²Sciex, Brea, CA
- MP 536 **A Standard Assessment of the Extracellular Vesicles' Purification Methods by Targeted Mass Spectrometry**; Tingting Wang^{1,2}; Kyle W Anderson^{1,2}; Illarion V. Turko^{1,2}; ¹NIST, Gaithersburg, MD; ²Institute for Bioscience and Biotechnology, Rockville, MD
- MP 537 **A Carrier-Assisted Targeted Mass Spectrometry Approach for Proteomics Analysis of Single Cells**; Tujin Shi¹; Matthew J. Gaffrey¹; Thomas L. Fillmore¹; Song Nie¹; Carrie D. Nicora¹; H. Steven Wiley¹; Karin D. Rodland¹; Tao Liu¹; Richard D. Smith¹; Wei-Jun Qian¹; ¹PNNL, Richland, WA
- MP 538 **An Objective Cross-Platform Comparison between MRM and PRM Based Quantitative Plasma Proteomic Workflows Reveals Similar Sensitivity and Reproducibility**; Vincent R. Richard¹; Andre M. LeBlanc¹; Christoph H. Borchers^{1,2,3,4}; ¹JGH Proteomics Centre, Lady Davis Institute, McGill University, Montreal, QC, Canada; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ³Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁴Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada
- PLANT "OMICS"**
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- MP 539 **Multi-omic Approach for Characterizing Plant Peptide Hormone Signaling Pathways That Regulate Cell Expansion**; Greg Sabat¹; Gregory A. Barrett-Wilt¹; Michael R. Sussman¹; ¹University of Wisconsin, Madison, WI
- MP 540 **Engineered Resistance to a Bean Fungal Disease against Proteins Found by Mass Spectrometry**; Bret Cooper; USDA-ARS, Beltsville, MD
- MP 541 **Analysis of Canadian Wheat Varieties Low Molecular Weight Glutenin Subunits Relative to Gluten Strength : A Genotype x Environment Study**; Dave Hatcher¹; Raymond Bacala¹; ¹Grain Research Lab, Canadian Grain Commission, Winnipeg, MB
- MP 542 **Investigation of Kinase-Substrate Networks in Photosynthetic Organisms**; Megan M. Ford¹; Alex Chao¹; Chris A. Broberg¹; Leslie M. Hicks¹; ¹University of North Carolina, Chapel Hill, NC
- MP 543 **The Proteomic Profile of Rice Mitosis under Drought Stress**; Paul A. Haynes¹; Yungi Wu¹; Mehdi Mirzaei¹; Dana Pascovici²; Brian J. Atwell³; ¹Dept of Chemistry and Biomolecular Sciences, Macquarie University, North Ryde, Sydney, Australia; ²Australian Proteome Analysis Facility, Macquarie University, North Ryde, Sydney, Australia; ³Dept of Biological Sciences, Macquarie University, North Ryde, Sydney, Australia
- MP 544 **Global Analysis of Native Protein Complexes in Cyanobacteria ATCC 51142 using Label-Free Quantitative Proteomic Profiling**; Uma Aryal¹; Victoria Hedrick¹; Tiago José Paschoal Paschoal Sobreira¹; Christina R Ferreira¹; Ding Ziyun²; Daisuke Kihara²; Louis Sherman³; ¹Bindley Bioscience Center, Purdue University, West Lafayette, IN; ²Department of Computer Science, Purdue University, West Lafayette, United Arab Emirates; ³Department of Biological Sciences, Purdue University, West Lafayette, IN
- MP 545 **Leaf Spray Mass Spectrometry for Soybean Metabolomics**; Troy Wood¹; Kevin Zemaitis¹; Daniel Szczepankiewicz¹; ¹University at Buffalo, Buffalo, NY
- MP 546 **Ion Mobility and High Resolution Mass Spectrometry of Centella asiatica Extracts – Characterization and Quantification of Phytochemical Constituents**; Armando Alcazar Magana¹; Maya Caruso²; Amala Soumyanath²; Joseph Quinn^{2,3}; Jan F. Stevens^{4,5}; Claudia S. Maier¹; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²Department of Neurology, Oregon Health & Science University, Portland, OR; ³Department of Neurology and Parkinson's Disease Research Education and Clinical Care Center, Portland, OR; ⁴Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; ⁵Linus Pauling Institute, Oregon State University, Corvallis, OR
- MP 547 **Evaluation of ETD, HCD and CID Fragmentation for Phosphoproteomics of Grape (Vitis vinifera L.) Berries**; Liping Yang¹; Satyanarayana Gouthu²; Laurent G. Deluc²; Claudia S. Maier^{1,3}; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²Department of Horticulture, Oregon State University, Corvallis, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR



MONDAY POSTERS

- MP 548 **Using Metabolomics to Uncover Metabolic Pathways Utilized in Nitrogen Stress and Plant-Microbe Interactions in Energy Sorghum**; Amy M. Shefflin¹; Jessica E. Prenni¹; Daniel P. Schachtman²; Rebecca Bart³; Thomas Brutnell³; Daniel Chitwood³; Asaph Cousins⁴; Jeffrey Dangl⁵; Ismail Dweikat²; Andrea Eveland³; Maria Harrison⁶; Stephen Kresovich⁷; Peng Liu⁸; Todd Mockler³; Susannah Tringe⁹; Arthur Zygierbaum²; ¹Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; ²University of Nebraska-Lincoln, Lincoln, NE; ³Donald Danforth Plant Science Center, St. Louis, MO; ⁴Washington State University, Pullman, WA; ⁵UNC-Chapel Hill, Chapel Hill, NC; ⁶Boyce Thompson Institute, Ithaca, NY; ⁷Clemson University, Clemson, SC; ⁸Iowa State University, Ames, IA; ⁹Joint Genome Institute-DOE, Walnut Creek, CA
- MP 549 **Proteomic Identification of BIK1 Direct Substrates that Mediate the Arabidopsis innate Immunity**; Peipei Zhu¹; Chuan-Chih Hsu¹; Pengchang Wang¹; Yanyan Du¹; Jian-Kang Zhu¹; W. Andy Tao¹; ¹Purdue University, West Lafayette, IN
- MP 550 **Paterno-Buchi (PB) Reaction Coupled with Tandem Mass Spectrometry for the Analysis of Plant Lipids and Their Isomers**; Leelyn Chong¹; Zheng Ouyang^{2,3}; Yu Xia^{2,3}; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, Indiana; ³Tsinghua University, Beijing, Beijing
- MP 551 **Investigation of Natural Products in Symbiotic Nitrogen-Fixing Root Nodules of *Datisca glomerata* by LC-MSn and Ion Tree Analysis using iTree**; Arpana Vaniya^{1,2}; Sajjan S. Mehta²; Kai Battenberg³; Alison Berry³; Oliver Fiehn²; ¹UC Davis Department of Chemistry, Davis, CA; ²West Coast Metabolomics Center, Davis, CA; ³UC Davis Department of Plant Sciences, Davis, CA
- MP 552 **Advances in the Use of *in vivo* Crosslinking and Immunoaffinity Purification-Mass Spectrometry to Provide Insights into Unconventional Protein Secretion**; Tricia C. Ho¹; Kevin Blackburn¹; John D. Williamson¹; Michael B. Goshe¹; ¹NC State University, Raleigh, NC
- MP 553 **Proteomic Analysis of H2S Induced Protein S-Sulfhydration in *Arabidopsis thaliana***; Yixiang Zhang^{1,2}; Xuhong Yu³; Hui Peng^{1,4}; David P. Giedroc^{1,4}; Scott D. Michaels³; Jonathan Trinidad^{1,2}; ¹Department of Chemistry, Indiana University, Bloomington, IN; ²Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; ³Department of Biology, Indiana University, Bloomington, IN; ⁴Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN
- MP 554 **GC-MS and UHPLC-HRMS Analysis of *Aechmea magdalenae* Rhizome against *E. coli* and *S. aureus***; Mirna Giron¹; Quintin Ferraris¹; Anima Ghosal¹; Dil Ramanathan²; ¹Kean University, Union, NJ; ²Kean University, Union, NJ
- MP 555 **Detecting the "Un-natural" in Natural Products**; Jimmy Yuk¹; Dhavalkumar Narendrabhai Patel²; Sukhdev Bangar³; Yun Wang Alelyunas¹; Jayne Kirk⁴; Giorgis Isaac¹; Mark Wrona¹; ¹Waters Corporation, Milford, MA; ²Waters Pacific Private Ltd, Singapore, Singapore; ³Waters Corporation, Beverly, MA; ⁴Waters Corporation, Wilmslow, UK
- MP 556 **Chemical Fingerprinting of Essential Oils from Conifer Needles by ESI/APPI FT-ICR Mass Spectrometry**; Omolara Mofikoya¹; Marko Mäkinen¹; Janne Jänis¹; ¹Department of Chemistry, University of Eastern Finland, Joensuu, Finland
- MP 557 **Divergence in Phenolic Secondary Metabolites and Tyrosine Hyperaccumulation among Populations in the *Inga umbellifera* clade (Fabaceae), a Tropical Tree**; Gordon C. Younkin¹; Dale L. Forrister¹; Gabrielle Ghabash¹; Phyllis D. Coley^{1,2}; Maria-Jose Endara¹; James A. Nicholls³; R. Toby Pennington⁴; Kyle G. Dexter³; Graham N. Stone³; Catherine A. Kidner⁴; Thomas A. Kursar^{2,5}; ¹University of Utah, Salt Lake City, UT; ²Smithsonian Tropical Research Institute, Panama City, Panama; ³University of Edinburgh, Edinburgh, UK; ⁴Royal Botanic Garden Edinburgh, Edinburgh, UK; ⁵University of Utah, Salt Lake City, UT
- MP 558 **Temporal Proteome and Metabolome Profiling of Water-Deficit Stress Responses in *Populus* Leaves**; Paul E. Abraham¹; Daniel A. Jacobson¹; Robert L. Hettich¹; Gerald A. Tuskan¹; Timothy J. Tschaplinski¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- MP 559 **Identifying and Characterizing Plant-Derived Cyclic Peptides via High Resolution LC-MS/MS**; Nicole C Parsley¹; Christine L Kirkpatrick¹; Leslie M Hicks¹; ¹University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC
- MP 560 **Comparison of Different Offline Fractionation Techniques for Label Free Proteome Profiling of *Arabidopsis* Leaf Tissue**; Julia Mergner¹; Lucia Guettler¹; Bernhard Kuster¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany
- MP 561 **Proteome Analysis of *Brachypodium distachyon* Leaves under Drought Stress with Timewise Variation**; Ozge Tatli¹; Bahar Sogutmaz Ozdemir²; Gizem Dinler Doganay¹; ¹Istanbul Technical University, Istanbul, Turkey; ²Yeditepe University, Istanbul, Turkey
- ### PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS I
- #### 562 - 592
- MP 562 **Evidence that the Polyglutamine Aggregation Inhibitor QBP1 Interacts with Monomeric Ataxin-3 at a Novel Site**; Patrick Knight¹; Theodoros Karamonos¹; Sheena E Radford¹; Alison E Ashcroft¹; ¹University of Leeds, Leeds, Yorkshire
- MP 563 **Assessing Conformational Heterogeneities of Beta-2 Microglobulin Pre-Amyloid Oligomers using Ion Mobility Mass Spectrometry**; Tyler Marcinko¹; Richard W Vachet¹; ¹University of Massachusetts-Amherst, Amherst, MA
- MP 564 **Time-Resolve Mass Spectrometry with a Micromixing Tee Applied to Kinetic Studies of Cd2+ Binding to Methallothionein-2A**; Shiyu Dong¹; Nicole Wagner¹; David H Russell¹; ¹Texas A&M University, College Station, TX
- MP 565 **Characterization of Biotherapeutics by Native SEC-MS: from Cysteine-linked Antibody Conjugates to Megadalton Protein Assembly**; Jia Dong¹; Suprit Deol¹; Feng Wang¹; Bryant Chau¹; Karla Henning¹; David Passmore¹; ¹Bristol-Myers Squibb, Redwood City, CA
- MP 566 **Interaction Proteomics on Glycine Receptor Interactome Reveal Novel Interactors: Implication in Inhibitory Neurotransmission in Brain Stem and Spinal Cord**; Sophie J.F. van der Spek¹; Frank Koopmans¹; Miguel A. Gonzalez-Lozano¹; Roel van der Schors¹; Ka Wan Li¹; August B. Smit¹; ¹CNCR, VU Amsterdam, Amsterdam, Noord Holland
- MP 567 **Investigating Additional Functions of BMV Capsid Protein by Mass Spectrometry**; Alexander D. Jacobs¹; Haley S. Hoover²; C. Cheng Kao²; David E. Clemmer²; ¹Indiana University, Bloomington, IN; ²Indiana University, Bloomington, IN
- MP 568 **Determining Ligand Interactions of Parvovirus with Fragment Antibodies and Transferrin Receptors using Charge Detection Mass Spectrometry**; Carmen Dunbar¹; Heather Callaway²; Colin Parrish²; Martin Jarrold¹; ¹Indiana University, Bloomington, IN; ²Cornell University, Ithaca, NY
- MP 569 **Separation and Quantification of Amyloid Beta Oligomers and Monomers Using a 2D-LC-MS/MS System**; Farid Jahouh¹; Herman Borghys²; Filip Cuyckens¹; Rob J Vreeken^{1,3}; ¹Discovery Sciences, Janssen Pharmaceutica, Beerse, Belgium; ²Neurosciences Department, Janssen Pharmaceutica, Beerse, Belgium; ³M&I Institute - Maastricht University, Maastricht, Netherlands



- MP 570 **Novel Protein-Protein Interactions with Specific Functional Domains of RNA Polymerase II;** Whitney Smith-Kinnaman¹; Asha Boyd¹; Nada Alakhras¹; Gabriela Mazur²; Lynn Bedard³; Amber Mosley¹; ¹Indiana University School of Medicine, Indianapolis, IN; ²Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³DePauw University, Greencastle, IN
- MP 571 **Using Native Top-Down ESI FTICR-MS to Characterize the Interaction of Tau Protein with Assembly Modulator CLR01;** Michael Nshanian¹; Joseph A Loo¹; Piriya Wongkongkathap¹; Gal Bitan¹; ¹UCLA, Los Angeles, CA
- MP 572 **Anti-apoptotic Bag-1S is Involved in Ubiquitin-Dependent Proteasomal Degradation by Forming a Complex with AAA ATPase, p97/VCP;** Sevilay Acar¹; Nisan Can¹; Tugba Kizilboga¹; Ozge Tatli¹; Gizem Dinler Doganay²; ¹Istanbul Technical University, Istanbul, Turkey; ²Istanbul
- MP 573 **Analysis of Oxygen Sensitive Nitrogenase Complexes using Native Mass Spectrometry;** Monika Tokmina-Lukaszewska¹; Natasha Pence¹; Rhesa Ledbetter²; Zhiyong Yang²; John Peters³; Lance Seefeldt²; Brian Bothner¹; ¹Montana State University, Bozeman, MT; ²Utah State University, Logan, UT; ³Washington State University, Pullman, WA
- MP 574 **The Effect of Protein Concentration and Metal Content on Calprotectin Oligomerization as Revealed by Native Electrospray Ionization Mass Spectrometry;** Boone M. Prentice¹; Benjamin A Gilston²; Kevin L. Schey²; Walter J Chazin²; Richard M. Caprioli²; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt University, Nashville, TN
- MP 575 **Identification of Interaction Partners of Protein Phosphatase 2A in Human Skeletal Muscle using Label Free Mass spectrometry;** divyasri damacharla¹; Zhengping Yi²; Xiangmin Zhang²; Danjun ma¹; Yue Qi¹; berhane seyoum¹; Abdullah mallisho¹; sorin Dragichi¹; Michael Caruso¹; ¹Wayne State University, Detroit, MI; ²Wayne State University, Detroit, MI
- MP 576 **Limited Charge Reduction Coupled IM-MS Reveals Distinct Models of Biopolymers Interaction between Protamine and Heparin;** Yunlong Zhao¹; Igor A. Kaltashov²; ¹University of Massachusetts Amherst, Amherst, MA; ²University of Massachusetts-Amherst, Amherst, MA
- MP 577 **Identification of the 'Readers' of Histone Modification by Combination of DNA-templated Peptide Probe and Mass Spectrometry Analysis;** Xue Bai¹; Congcong Lu²; Shanshan Tian¹; Guijin Zhai¹; Kai Zhang^{1,2}; ¹Tianjin Medical University, Tianjin, Tianjin; ²Nankai University, Tianjin
- MP 578 **Comparative Interactome Analysis of Multidrug-Resistant and Sensitive Pathogenic Bacteria Strains of Acinetobacter baumannii ;** Xuefei Zhong¹; Xia Wu¹; Juan D. Chavez¹; Devin K Schweppe¹; Arti T Navare¹; Jimmy K Eng¹; James E Bruce¹; ¹University of Washington, Seattle, WA
- MP 579 **Screening and Characterization of Nanobody-ABC-transporter Complexes using High-Mass Matrix-Assisted Laser Desorption/Ionization-Mass Spectrometry;** Martin Köhler¹; Camilo Perez²; Kaspar Locher²; Renato Zenobi¹; ¹ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland; ²ETH Zurich, Institute of Molecular Biology and Biophysics, Zurich, Switzerland
- MP 580 **Investigation of GTP-Dependent K-Ras Oligomerization Using Native Top-Down Ultraviolet Photodissociation Mass Spectrometry;** M. Rachel Mehaffey¹; Michael B. Cammarata¹; Christopher L. Schardon²; Walter Fast³; Jennifer S. Brodbelt¹; ¹Department of Chemistry, University of Texas at Austin, Austin, TX; ²Graduate Program in Biochemistry, University of Texas at Austin, Austin, TX; ³Division of Chemical Biology and Medicinal Chemistry, College of Pharmacy, University of Texas at Austin, Austin, TX
- MP 581 **Interaction of Transcription Factor TEAD and Its DNA Response Element from C-MYC Promoter Studied by Structural Mass Spectrometry;** Ruzena Liskova^{1,2}; Lukas Slavata^{1,2}; Daniel Kavan^{1,2}; Karel Valis^{1,2}; Petr Man^{1,2}; Petr Novak^{1,2}; ¹BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; ²Faculty of Science, Charles University, Prague, Czech Republic
- MP 582 **Determination of the Heparin-Binding Sites of RPTP-LARs Via HRFP-FPOP and LC-MS/MS;** Charles Mobley¹; Pradeep Prabhakar²; Chelsea Suppinger¹; Kelley Moremen²; Joshua Sharp¹; ¹University of Mississippi, Oxford, MS; ²University of Georgia, Athens, GA
- MP 583 **Quantifying the Effects of Membrane Composition on Protein-Glycolipid Interactions Using Nanodiscs and Proxy Ligand ESI-MS;** Ling Han¹; Elena Kitova¹; John Klassen¹; ¹University of Alberta, Edmonton, AB, Canada
- MP 584 **Native Mass Spectrometry to Identify Stoichiometries and Stability of Protein-Ligand Complexes;** Sabine Wittig¹; Marius Rutkauskas²; Ralf Seidel²; Carla Schmidt¹; ¹IWE ZIK HALOmern Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany; ²Institute of Experimental Physics I Universität Leipzig, Leipzig, Germany
- MP 585 **Elucidating Cellular Locales by Crosslinking Mass Spectrometry;** Richard A. Scheltema^{1,2}; Fan Liu^{1,2}; Oleg Klykov^{1,2}; Sibel Bayrak^{1,2}; Barbara Steigenberger^{1,2}; Domenico Fasci^{1,2}; Albert J. R. Heck^{1,2}; ¹Utrecht University, Utrecht, Netherlands; ²Netherlands Proteomics Center, Utrecht, Netherlands
- MP 586 **Dynamic Protein Interactions and Post-Translational Modifications in Monocytes;** Annika Frauenstein¹; Matthias Mann¹; Felix Meißner¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- MP 587 **MS Study of Zinc-Binding to Mutant Forms of Amyloid-Beta Provide an Insight on the Early Mechanisms of Familial Alzheimer's Disease;** Maria I. Indeykina^{1,2,3}; Alexey S. Kononikhin^{1,2,3}; Igor A. Popov^{1,2,3}; Aleksandra A. Kulikova⁴; Sergey A. Kozin⁴; Eugene (Evgeny) Nikolaev^{2,3,5}; ¹Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; ²Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; ³Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ⁴Engelhardt Institute of Molecular Biology, Moscow, Russia; ⁵Skolkovo institute of science and technology, Skolkovo, Russia
- MP 588 **Analysis of a Reconstituted, Non-Covalent Type III-A CRISPR-Cas Complex using Native Mass Spectrometry;** Tina Y. Liu^{1,2,3,4}; Anthony T Iavarone^{3,4}; Jennifer A. Doudna^{1,2,3,5,6}; ¹Department of Molecular and Cell Biology, University of California, Berkeley, CA; ²Howard Hughes Medical Institute, University of California, Berkeley, CA; ³California Institute for Quantitative Biosciences, University of California, Berkeley, CA; ⁴Department of Chemistry, University of California, Berkeley, CA; ⁵Innovative Genomics Initiative, University of California, Berkeley, CA; ⁶MBIB Division, Lawrence Berkeley National Laboratory, Berkeley, CA
- MP 589 **Mapping the HLA Antibody Interaction with Blue Paint;** William Hildebrand¹; Virginie Sjoelund¹; ¹OUHSC, Oklahoma City, OK
- MP 590 **Development of an MS Approach for Characterizing Intracellular Proteins Interacting with a G Protein-Coupled Receptor Captured using Laser-Induced Photo-Activation;** Chen Qian^{1,2}; Melinda Hauser²; Tyler King²; Jeffrey Becker²; Robert Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN
- MP 591 **High Throughput, Label- and Immobilization-Free Screening of Human Milk Oligosaccharides against Lectins;** Amr El-Hawiet^{1,2}; Yajie Chen¹; Km Shams-Ud-Doha¹; Elena N. Kitova¹; John S. Klassen¹; ¹Alberta Glycomics Centre and Department of Chemistry,



- MP 592 **Native Mass Spectrometry Reveals Endogenous Stoichiometric Control Governing Protein Complexation in Metabolism: A Case Study of Glycolytic Enzyme Triosephosphate Isomerase;** Luis F. Schachner¹; Benjamin Des Soye²; Nicole A Haverland²; Josiah Hutton²; Owen Skinner²; Michael Jewett²; Philip Compton²; Neil L Kelleher²; ¹Northwestern University, Evanston, IL; ²Northwestern University, Evanston, IL

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- MP 593 **Large-scale Characterization and Quantitation of Citrullinated Proteins Involved in Restenosis by HCD Product Ion Triggered EThcD Mass Spectrometry;** Yatao Shi¹; Zhengwei Chen²; Qing Yu³; Bowen Wang⁴; Matthew Glover⁵; Xudong Shi⁶; Lian-wang Guo⁴; Craig K. Kent⁴; Lingjun Li^{5,7}; ¹Madison, Wisconsin; ²Chemistry Department, University of Wisconsin-Madison, Madison, WI; ³Pharmacy School, University of Wisconsin-Madison, Madison, WI; ⁴Davis Heart and Lung Research Institute, The Ohio State University, Columbus, OH; ⁵School of pharmacy, University of Wisconsin-Madison, Madison, WI; ⁶Department of Surgery, University of Wisconsin-Madison, Madison, WI; ⁷Department of chemistry, University of Wisconsin-Madison, Madison, WI
- MP 594 **MS-compatible Subcellular Fractionation Protocol based on Phase Transfer Surfactants;** Takeshi Masuda¹; Naoyuki Sugiyama²; Sumio Ohtsuki¹; Yasushi Ishihama²; ¹Kumamoto University, Kumamoto, Japan; ²Kyoto University, Kyoto, Japan
- MP 595 **A Proteomics Approach to Characterize Trace Host Cell Protein Impurities in Drug Substance and Guide Purification Process Development;** Yu Zhou¹; Sushmita Mimi Roy¹; ¹BioMarin Pharmaceutical Inc., Novato, CA
- MP 596 **Proteomic Analysis Identifies Novel Regulators of the ade6-M26 Meiotic Recombination Hotspot;** Aaron Storey¹; Stephanie Byrum¹; Mari K. Davidson¹; Alan J Tackett¹; Sam Mackintosh¹; Wayne P. Wahls¹; ¹University of Arkansas for Medical Sciences, Little Rock, AR
- MP 597 **Microfluidic Nanoliter Sample Preparation Enables Deep Proteome Analysis of 10 Cells;** Ying Zhu¹; Paul D Piehowski²; Rui Zhao²; Yufeng Shen²; Ronald J Moore²; Weijun Qian²; Richard D. Smith²; Ryan Kelly²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA
- MP 598 **Epitope Identification and Affinity Quantification of β Amyloid Specific Antibodies using Online SPR-Biosensor- ESIMS;** Loredana Mirela Lupu^{1,2}; Hendrik Rusche^{3,4}; Zdenek Kukacka³; Yannick Baschung^{2,3}; Marry Murphy⁵; Jeff Bornheim⁵; Michael Przybylski^{3,4}; ¹Steinbeis Center for Biopolymer Analysis & Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; ²Proteom Zentrum Rostock, Institut für Immunologie, Universitätmedizin Rostock, Rostock, Germany; ³Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; ⁴University of Konstanz, Department of Chemistry, Konstanz, Germany; ⁵Reichert-Ametek Technologies, Buffalo, NY
- MP 599 **Database Independent Protein Sequencing (DiPS) Enables Full-Length de-novo Protein and Antibody Sequence Determination;** Alon Savidor¹; Rotem Barzilay¹; Dalia Elinger¹; Yosef Yarden²; Moshit Lindzen²; Alexandra Gabashvili¹; Ophir Adiv Tal¹; Yishai Levin¹; ¹The Nancy and Stephen Grand Israel National Center for Personalized Medicine, Weizmann Institute of Science, Rehovot, Israel; ²Department of Biological Regulation, Weizmann Institute of

- Science, Rehovot, Israel
- MP 600 **Optimization of a Promising Sample Preparation Protocol, Tube-Gel, for High Throughput Quantitative Proteomics;** Leslie Muller¹; Luc Fornecker¹; Alain Van Dorsselaer¹; Sarah Cianferani¹; Thierry Rabilloud²; Christine Carapito¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; ²Laboratoire de Chimie et Biologie des Métaux, UMR 5249, iRTSV/LCBM, CEA, Grenoble, France
- MP 601 **'Boxcar' Method Enables Single Shot Proteomics at a Depth of 10,000 Proteins in 100 Minutes on a Hybrid Quadrupole-Orbitrap Instrument;** Florian Meier¹; Philipp E Geyer^{1,2}; Juergen Cox¹; Matthias Mann^{1,2}; ¹Max-Planck Institute of Biochemistry, Martinsried, Germany; ²NNF Center for Protein Research, Copenhagen, Denmark
- MP 602 **Ion 'Supercharging' for Improving Bottom-Up Protein Analysis by Liquid-Chromatography Mass Spectrometry;** Muhammad Zenaidee¹; William A. Donald²; Mark J. Raftery²; Sydney Liu Lau³; ¹Kensington, NSW; ²University of New South Wales, Sydney, Australia; ³Bioanalytical Mass Spectrometry, Sydney, NSW
- MP 603 **Scanning the Human Proteome for Multi-cistronic Genes;** Samuel Smukowski¹; Xiaofei Du²; Daniel PH Pastor²; Jack D Godfrey²; Eshaan Rao²; Christopher M Gomez²; Jeffrey N Savas³; ¹Northwestern University, Chicago, IL; ²University of Chicago, Chicago, IL; ³Northwestern University, Chicago, IL
- MP 604 **Isolated Pseudomonas aeruginosa from Mining Site: Proteome Changes Due to the Copper;** Cristiano José de Andrade^{1,2}; Meriellen Dias^{1,2}; Lidiane Maria de Andrade^{1,2}; Camila Delarmelina³; Marta Cristina Teixeira Duarte³; Maria Anita Mendes^{1,2}; Claudio Augusto Oller do Nascimento^{1,2}; ¹Universidade de São Paulo - USP, Sao Paulo, South America; ²Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil; ³Chemical, Biological and Agricultural Pluridisciplinary Research Center (CPQBA); University of Campinas - Brazil, Campinas, Brazil
- MP 605 **Diethylaminoethyl Sepharose (DEAE-Sepharose) Microcolumn for Glycopeptides Enrichment;** He Zhu¹; Cheng Ma²; Peng George Wang²; ¹Atlanta, GA; ²Georgia State University, Atlanta, GA
- MP 606 **Analysis of Specific Synaptic Proteomes in Rodent Models of Autism Spectrum Disorder;** Yi-Zhi Wang¹; Samuel N Smukowski¹; Kira A Cozzolino¹; Jeffrey N Savas¹; ¹Northwestern University, Chicago, IL
- MP 607 **Proteome-wide Characterization of Metabolic Drugs AICAR and Metformin by Thermal Shift Assays;** Katherine A Overmyer¹; Harald Marx¹; Alex S Hebert¹; Michael S Westphall¹; Joshua J. Coon¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 608 **Comparison of Proteomic Profile of the Aspergillus niger Fungus (ATCC 11414 and Savage) Growing in Presence of Copper;** Meriellen Dias^{1,2}; Lidiane Maria de Andrade^{1,2}; Enrique Eduardo Rozas Sanchez^{1,2}; Maria Anita Mendes^{1,2}; ¹Universidade de São Paulo - USP, Sao Paulo, South America; ²Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil
- MP 609 **SAVControl: A Computational Framework for Quality Control of Variant Peptide Detection in Shotgun Proteomics;** Xinpei Yi¹; Bo Wang²; Zhiwu An¹; Fuzhou Gong¹; Jing Li²; Yan Fu¹; ¹Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China; ²Department of Bioinformatics and Biostatistics, School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, Shanghai, China
- MP 610 **Automated Reproducible High-Throughput Proteome Analysis using Magnetic HILIC Microparticles;** Stoyan Stoychev¹; Previn Naicker¹; Isak Gerber¹; Sipho Mamputha¹; Justin Jordaan²; ¹CSIR Biosciences, Pretoria, Gauteng; ²ReSyn Biosciences, Pretoria, South Africa



- MP 611 **Trinity P1 Mixed Mode Chromatography Enables Streamlined MS Compatible Orthogonal Peptide Fractionation**; Peng Yu¹; Mathias Wilhelm¹; Daniel P Zolg¹; Xuefei Sun²; Andreas Huhmer³; Bernhard Kuster^{1,4,5}; ¹Technical University of Munich, Freising, Germany; ²Thermo Fisher Scientific, Sunnyvale, CA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Center for Integrated Protein Science Munich, Freising, Germany; ⁵Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany
- MP 612 **Project Julienne: Improved Quantitative Detection of Protein Isoforms, Post Translational Modifications and Total Proteome Coverage**; Thomas Clark¹; Greg Stacey¹; Nikolay Stoyanov¹; Leonard Foster¹; ¹UBC, Vancouver, BC, Canada
- MP 613 **High-throughput Orthogonal Validation of Plasma Membrane-Associated Networks by Differential Centrifugation**; Emmanuel E Ojefua¹; Vincent C Chen¹; ¹Brandon University, Department of Chemistry, Brandon, MB
- MP 614 **The Loss-Less and Nano-Flow SPIDER Fractionator for High Sensitivity, High Coverage Proteomics**; Nils A. Kulak¹; Philipp E Geyer²; Garwin Pichler¹; Matthias Mann²; ¹PreOmics, Planegg/Martinsried, Bavaria; ²Max Planck Institute of Biochemistry, Martinsried, Germany
- MP 615 **Progress in Electrochemical Reduction of Disulfide Bonds in MS Proteomics**; Jean-Pierre Chervet¹; Pablo Sanz de la Torre¹; Hendrik-Jan Brouwer¹; Nico Reinhoud¹; Martin Eysberg²; ¹Antec Scientific, Zoeterwoude, Netherlands; ²Antec Scientific (USA), Boston, MA
- MP 616 **Highly Selective and Large Scale Mass Spectrometric Analysis of 4-Hydroxynonenal Modification via Fluorous Derivatization and Fluorous Solid-Phase Extraction**; Haojie Lu; , Shanghai, Shanghai
- MP 617 **Creation and Improvement of Software Tools for Kinetic Proteomics Analysis**; Bradley Naylor¹; Richard H Carson²; Marcus Hadfield²; John C Price²; ¹Brigham Young University, Provo, UT; ²Brigham Young University, Provo, UT
- MP 618 **Infrared Laser Desorption Capture Coupled with Ion Mobility-Mass Spectrometry and Chemometric Deconvolution for Analysis of Biological Tissues**; Michael E. Pettit¹; Raul A. Villacoba¹; Matthew R. Brantley¹; Fabrizio Donnarumma²; Kermit K. Murray²; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²Louisiana State University, Baton Rouge, LA
- MP 619 **Aff-BAMS: A High Throughput Immunoaffinity Enrichment Assay with Detection by LAESI MS and MALDI MS**; Callee Walsh¹; Erin H. Seeley¹; Vladislav Bergho²; ¹Protea Biosciences, Morgantown, WV; ²Adeptrix Corp, Beverly, MA
- MP 620 **Evaluating the Performance of an Automated, Inexpensive Hood Robot by Developing an Open-Source, Python-Scripted In-Gel Digestion Workflow for Bottom-Up Proteomics**; Roasa Mehmood¹; Ryan D. Leib¹; Allis S. Chien¹; Christopher M. Adams¹; ¹Stanford University Mass Spectrometry, Stanford, CA
- MP 621 **Reference Materials for Proteomic Investigations**; David M Bunk¹; Ashley Beasley-Green²; Candice Johnson²; Lisa E. Kilpatrick²; Mark S. Lowenthal²; Karen W. Phinney²; ¹NIST, Gaithersburg, MD; ²National Institute of Standards and Technology, Gaithersburg, MD
- MP 622 **Proteome Signal Amplification Using TMT Multiplexing and a Carrier/Reference Strategy**; Paul M. Stemmer¹; Nicholas J. Carruthers²; Joseph A. Caruso¹; D. Randy Armant¹; Sascha Drewlo¹; ¹Wayne State University, Detroit, MI; ²Wayne State University, Detroit, MI
- MP 623 **A Synergistic Approach: Combining Label-Free Proteomics and MRM Techniques in a Single Method to Advance Health Care**; Bruce E. Wilcox¹; Ryan W. Benz¹; Phong Cun¹; William F. Smith¹; ¹Applied Proteomics, San Diego, CA
- MP 624 **Investigating Protease Multiplexing to Improve Sequence Coverage in Bottom-Up Proteomics**; Jan Schrader¹; Assa Yeroslaviz¹; Anja Wehner¹; Juergen Cox¹; Nagarjuna Nagaraj¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- MP 625 **Identification of High pI-High Charge Peptides Using Capillary Electrophoresis Mass Spectrometry**; Tatiana N. Boronina¹; Robert N. Cole²; Robert N. O'Meally¹; ¹Johns Hopkins School of Medicine, Baltimore, MD; ²Johns Hopkins University School of Medicine, Baltimore, MD
- MP 626 **Mapping of T-Cell Surface N-Glycosylation**; Paul Kodama¹; Mirna Mujacic¹; Tom Kowski¹; Ken Prentice¹; ¹Juno Therapeutics, Seattle, WA
- MP 627 **Capillary Electrophoresis – Mass Spectrometry Analysis of Histatin 5 and Its Analogs**; Yan Wang¹; Svetlana P. Ikononova²; Amy J. Karlsson²; Fahim C. Zarrin³; James Xia³; ¹Proteomics Core Facility, University of Maryland, College Park, MD; ²Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD; ³CMP Scientific, Corp., Brooklyn, NY
- MP 628 **An Automated Online Sample Preconcentration Platform for Bottom-Up Proteomics by Capillary Electrophoresis-Mass Spectrometry**; Zhenbin Zhang¹; Elizabeth Peuchen¹; Norman J Dovichi¹; ¹University of Notre Dame, Notre Dame, IN
- MP 629 **Open Sesame: Proteomics and Lipidomics of Oil and Fat Illuminants from Archaeological Lamps**; Anna Shevchenko¹; Yimin Yang²; Andrea Schuhmann¹; Bo Wang³; Changsui Wang²; Andrej Shevchenko¹; ¹MPI of Mol Cell Biology and Genetics, Dresden, Saxony; ²University of Chinese Academy of Sciences, Beijing, China; ³Xinjiang Uygur Autonomous Region Museum, Ürümqi, China
- MP 630 **Characterizing the Inhibitory Postsynaptic Proteome Directly from Mouse Brain Tissue using *in vivo* BiOLD Proximity Labeling and label Free Quantitation**; Erik J. Soderblom¹; Akiyoshi Uezu²; M. Arthur Moseley¹; Scott H. Soderling²; ¹Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham, NC; ²Department of Cell Biology, Duke University School of Medicine, Durham, NC
- MP 631 **Proteomic of microalgae *Chlorella kessleri* Cultivation under Stressed Condition Induced by Copper Ions**; Lidiane Maria Andrade^{1,2}; Meriellen Dias^{1,2}; Cristiano José Andrade^{1,2}; Maria Anita Mendes^{1,2}; Claudio Augusto Oller do Nascimento^{1,2}; ¹Universidade de São Paulo - USP, Sao Paulo, South America; ²Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil
- MP 632 **Evaluation of a Modified Q Exactive HF for Shotgun Proteomics**; Christian Kelstrup¹; Dorte B Bekker-Jensen¹; Tabiwan Arrey²; Alexander Harder²; Jesper V. Olsen¹; ¹CPR, University of Copenhagen, Copenhagen, Denmark; ²Thermo Fisher Scientific, Bremen, Germany

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- MP 633 **Utilizing an Accurate Mass and Retention Time Library to Facilitate Bio-Marker Discovery in the Human Cerebrospinal Fluid Proteome**; Cole Michel¹; Richard Reisdorff¹; Enrique Alvarez¹; Vadiraja Bhat²; Paul Goodley³; Nichole Reisdorff¹; ¹University of Colorado Anschutz Medical Campus, Aurora, CO; ²Agilent Technologies, Inc, Wilmington, DE; ³Agilent Technologies, Inc., Wilmington, DE
- MP 634 **Relative Protein Quantification of a Contrived Mixture with Fusion MS2 and MS3-SPS TMT10-Plex Data**; Candace R. Guerrero¹; Todd W. Markowski²; Alan J. Zimmerman²; Kristin L. M. Boylan¹; Susan K. Van Riper¹; Leeann Higgins²; Amy P. N. Skubitz¹; Timothy Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²University of Minnesota, St. Paul, MN



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- MP 635 **Protein Isoform Quantitation in Complex Proteomic Data**; Casimir Bamberger¹; Salvador Martínez-Bartolomé¹; Miranda Montgomery¹; Sandra Pankow¹; John D. Hulleman¹; Jeffery W. Kelly¹; Clara Moon¹; Dennis Wolan¹; John R. Yates III¹; ¹The Scripps Research Institute, La Jolla, CA; ²University of Texas Southwestern Medical Center, Dallas, TX
- MP 636 **Post Immuno-Enrichment On-Bead Digestion for Protein Quantification using immuno-MALDI (iMALDI)**; Huiyan Li¹; Robert Popp¹; Bjorn Frohlich¹; Christoph H. Borchers^{1,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- MP 637 **Absolute Quantification using Targeted Mass Spec Assays with Panorama and Skyline**; Nicholas Shulman¹; Josh Eckels²; Vagisha Sharma¹; Daniel S. Spellman³; Kristin Wildsmith⁴; Shadi Toghi Eshghi⁴; Jacob D Jaffe⁵; Michael J MacCoss¹; Brendan MacLean¹; ¹University of Washington, Department of Chemistry, Seattle, WA; ²LabKey, San Diego, CA; ³Merck & Co., West Point, PA; ⁴Genentech, Inc, South San Francisco, CA; ⁵Broad Institute, Cambridge, MA
- MP 638 **SPEAQ: A Software Tool for Absolute Protein Quantitation Based on Peptide Quantitative Efficiency Learning**; Qiang Zhi Gao¹; Cheng Chang²; Yan Fu¹; Hong Xiao Qian²; Ping Yun Zhu²; ¹National Center for Mathematics and Interdisciplinary Sciences, Key Laboratory of Random Complex Structures and Data Science, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China; ²State Key Laboratory of Proteomics, National Center for Protein Sciences Beijing, Beijing Proteome Research Center, National Engineering Research Center for Protein Drugs, Beijing, China
- MP 639 **Elaboration towards the Regulatory Mechanism of Phase Shift in Clostridium acetobutylicum with a Combinational Strategy of Omics**; Nannan Kong^{1,2}; Jingjing Zhao³; Qingfei Pan^{1,2}; Xiaomin Lou¹; Jin Zi²; Lin Wu¹; Yan Ren²; Quanhui Wang¹; Siqi Liu²; ¹Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; ²BGI-Shenzhen, Shenzhen, China; ³Diabetes and Obesity Center, U of L, Louisville, KY
- MP 640 **A Silk Road to Modern Translational Proteomics – SOPs based Comprehensive Proteome Profiling and Reproducible Quantitation**; Yue Xuan¹; David Sarracino²; Sebastien Gallien³; Scott Peterman²; Pedro Navarro¹; Heather Sumner⁴; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific BRIMS Center, Cambridge, MA; ³Thermo Fisher Scientific, Courtaboeuf, France; ⁴Thermo Fisher Scientific, San Jose, CA
- MP 641 **Dual and Triple Reporter Ion Combinatorial Isobaric Reagents: 16-Plex and Beyond**; Craig Braun^{1,2}; Brian K Erickson^{2,3}; Gregory H Bird⁴; Steve P Gygi³; ¹Harvard Medical School, Boston, MA; ²IQ Proteomics, LLC, Brookline, MA; ³Harvard Medical School, Boston, MA; ⁴Dana Farber Cancer Institute, Boston, MA
- MP 642 **Isobaric Tag-Based Multi-Dimensional Quality Assessment Standards for SPS-MS3 Analyses: Maximizing Quantifications, while Minimizing Interference**; Joao A Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA
- MP 643 **Multiplex Quantitative Analysis using NeuCode SILAC Metabolic Labeling of Signaling Protein Targets**; Ryan Bomgardner¹; Kratika Singhal¹; Bhavin Patel¹; Rosa Viner²; Seema Sharma³; Juergen Cox⁴; Joshua Coon⁵; JOHN C. ROGERS¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Max Planck Institute of Biochemistry, Martinsried, Germany; ⁵University of Wisconsin, Madison, WI
- MP 644 **Combined Proteomic and RNA Expression Analysis of Laser Ablation Extracted Tissue**; Chao Dong¹; Kelin Wang¹; Fabrizio Donnarumma¹; Scott W. Herke¹; Michael E. Pettit²; Touradj Solouki²; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA; ²Baylor University, Waco, TX
- MP 645 **Optimization of Multi-notch MS3 Technique for Accurate Quantification with Dimethyl Amino Acid-based Isobaric Tags**; Yusi Cui¹; Qing Yu²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- MP 646 **A Rapid Digestion Protocol for the Preparation of Complex Proteomic Samples**; Kevin Cook¹; Sergei Saveliev¹; Marjeta Urh¹; Michael M Rosenblatt¹; ¹Promega Corporation, Madison, WI
- MP 647 **Active Enzyme Characterization using a Two-Dimensional Isobaric Labeling Activity-Correlated Quantitative Proteomics Platform(2D-TMT-ACPP)**; Hongyan Ma¹; Toni Woodard²; Si Wu²; ¹Oklahoma University, Norman, OK; ²University of Oklahoma, Norman, OK
- MP 648 **IonStar-Mine: Reproducible, Fractionation-Free Measurement of 8000+ Unique Proteins in 100 Biological Samples with High Accuracy, Precision and <1% Missing Data**; Shichen Shen¹; Jun Li¹; Xiaomeng Shen²; Chengjian Tu¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Amgen, South San Francisco, CA
- MP 649 **Measuring Mitochondrial Protein Expression by Repeated Reinterrogation of LC-High Resolution Full Scan MS Datasets**; Caroline Kinter¹; Zachary Young¹; Luke Szveda¹; Michael Kinter¹; ¹Oklahoma Medical Research, Oklahoma City, OK
- MP 650 **MIKE: A Peptide-Terminal Labeling Strategy for Precision Quantitative (meta)Proteomics**; Jacob Waldbauer¹; Lichun Zhang¹; Adriana Rizzo¹; ¹University of Chicago, Chicago, IL
- MP 651 **Novel Tagging Strategies for a Modified cPILOT Workflow with Higher Sample Multiplexing Capabilities**; Bushra Amin¹; Renā A.S. Robinson¹; ¹University of Pittsburgh, Pittsburgh, PA
- MP 652 **Method for Measuring Protein Digestion Efficiency**; Carmen Fernandez-Metzler¹; Bonnie Baker¹; Richard King¹; ¹PharmaCadence Analytical Services, LLC, Hatfield, PA
- PROTEOMICS: TOP DOWN ANALYSIS I**
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- MP 653 **Online nano-2DLC Meets Top-Down MS: WCX/a*xm/ RPLC UVPD-HRMS Analysis of Histone Proteoforms**; Andrea Gargano¹; Jared B Shaw²; Mowei Zhou²; Nikola Tolic²; Thomas Fillmore²; Ronald J Moore²; Ljiljana Pasa-Tolic²; ¹Center for Analytical Chemistry Amsterdam, Amsterdam, Netherlands; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Earth and Biological Sciences Directorate, Richland, WA
- MP 654 **Characterization of Histone Proteoforms Using Linear and Nonlinear Ion Mobility Separations with Electron Transfer Dissociation**; Pavel Shliha¹; Matthew Baird²; Mogens Nielsen¹; Vladimir Gorshkov¹; Andrew P. Bowman²; Julia L. Kaszycki²; Gordon A Anderson³; Todd D. Williams⁴; Ole N. Jensen¹; Alexandre A. Shvartsburg²; ¹University of Southern Denmark, Odense, Denmark; ²Wichita State University, Wichita, KS; ³GAA Custom Engineering, LLC, Benton City, WA; ⁴University of Kansas, Lawrence, KS
- MP 655 **Automatic Selection of Discriminative Top-Down Mass Spectra with Diagno-Top: Application to the Differentiation of Bacterial Pathogens**; Diogo Borges Lima¹; Mathieu Dupré¹; André R F Silva²; Paulo Costa Carvalho²; Julia Chamot-Rooke¹; ¹Structural Mass Spectrometry and Proteomics Unit CNRS USR2000 Mass Spectrometry for Biology, Paris, France; ²Computational Mass Spectrometry & Proteomics Group, Carlos Chagas Institute, Curitiba, Paraná, Brazil, Curitiba, Brazil
- MP 656 **“Active” Fungal Classification Utilizing Top-Down Proteomics**; Toni Woodard¹; Zhe Wang¹; Hongyan Ma¹;



- Monica Stevenson¹; Si Wu¹; ¹University of Oklahoma, Norman, OK
- MP 657 **Top-down Proteomics of Sarcomeres in Muscle-related Diseases**; Wenxuan Cai¹; Zachery R Gregorich¹; Ziqing Lin¹; Zachary L Hite¹; Takushi Kohmoto¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 658 **High-Throughput Screening of Proteoform-Specific Binding of a Chemical Library Using a 24-plex Emitter Array Chip**; Geuncheol Gil¹; Pan Mao¹; Daojing Wang¹; ¹Newomics Inc., Emeryville, CA
- MP 659 **Increasing Dynamic Range and Sample Insight for Top-Down Proteoform Profiling Analysis Using Data-Dependent MS/MS Experiments**; Pierre-Olivier Schmit¹; Hans J.C.T. Wessels²; Marshall W. Bern³; Stephanie Kaspar-Schoenefeld⁴; Gary Kruppa⁵; ¹Bruker France, Wissembourg, France; ²Radboud Proteomics Center, Radboud University, Nijmegen, Netherlands; ³Protein Metrics Inc., San Carlos, CA; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵Bruker Daltonics, Billerica, MA
- MP 660 **A Multi-Modal Proteomics Strategy for Characterizing *in vitro* and *in vivo* p53 Modforms**; Caroline J DeHart¹; Luca Fornelli¹; Deepesh Agarwal²; Jacek W Sikora¹; Dan Lu²; Philip D Compton¹; Paul M Thomas¹; Galit Lahav²; Jeremy Gunawardena²; Neil L Kelleher¹; ¹Proteomics Center of Excellence, Northwestern University, Evanston, IL; ²Harvard Medical School, Boston, MA
- MP 661 **Top-down Online Electrospray Nano-Liquid Chromatography Orbitrap tandem Mass Spectrometry for Large Protein Identification in Cell Lysates**; Atim Atte Enyenihi¹; Jason Neil²; Mark Fisher^{1,3}; ¹ARUP Laboratories, Salt Lake City, UT; ²Thermo Fisher Scientific, Cambridge, Massachusetts; ³University of Utah, Salt Lake City, UT
- MP 662 **Simultaneous Label-free Quantitation of Proteoforms, Proteoform Ratios, and Total Protein up to 80kDa Split across Physiochemical Multidimensional Space**; John R Corbett^{1,2}; Daniel A Plymire¹; Casey E Wing¹; William S Phipps¹; Steven M Patrie^{1,2}; ¹UT Southwestern, Dallas, TX; ²UT Dallas, Richardson, TX
- MP 663 **Higher Resolution in Top-Down Proteomics of Histones using Submicrometer Particles and Slip Flow**; Yiyang Zhou¹; Ximo Zhang¹; Luca Fornelli²; Philip Compton²; Neil L Kelleher²; Mary Wirth¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN; ²Northwestern University, Evanston, IL
- MP 664 **Intelligent Data Acquisition Strategies to Generate a Comprehensive Map of Intact Proteoforms in Budding Yeast using Deep Top-Down Sequencing**; Luca Fornelli¹; Kristina Srzentic¹; Timothy K. Toby¹; Bryan P. Early¹; Peter F. Doubleday¹; Ryan T. Fellers¹; Philip D. Compton¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
- MP 665 **Elucidation of Experimental Fragmentation Parameters Required for High-Throughput Proteoform Interrogation of Myelin Basic Protein**; William S Phipps¹; John R Corbett¹; Casey E Wing¹; Lacey Purdue¹; Daniel A Plymire¹; Steven M Patrie¹; ¹University of Texas Southwestern Medical Center, Dallas, TX
- SMALL MOLECULES: QUANTITATIVE ANALYSIS I**
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- MP 666 **Chemical Analysis of ENDS vapor by LC/MS/MS-based Methodology**; Berk Oktem¹; Charles A. Moran¹; Samantha I Wickramasekara¹; ¹US FDA, Silver Spring, MD
- MP 667 **Evaluation of THERMAL HISTORY of THERMOPLASTIC RESINS by THERMAL DESORPTION and PYROLYSIS COMBINED with DART-MS (TDP/DART-MS)**; Chikako Takei¹; Kenichi Yoshizawa¹; ¹BioChromato, Inc., Fujisawa, Japan
- MP 668 **A Novel Approach to Minimize the Matrix Effect in the LC-MS/MS Method for Quantitation of N-(2-Hydroxyethyl) succinimide in Human Urine**; Dawei Zhou¹; Shaoting Zhang¹; Mohamed Osman¹; Xinping Fang¹; ¹WuXi AppTec, Plainsboro, NJ
- MP 669 **HPLC Tandem Mass Spectrometric Quantitation of DNA-binding Polyamides in Cell Lysate**; Shanshan Guan¹; Maria José Scuderi¹; Benjamin J. Bythell¹; James K. Bashkin¹; ¹University of Missouri-St. Louis, St. Louis, MO
- MP 670 **Selective Derivatization of Penicillamine Using DTNB: Improved Matrix Stability and LC-MS/MS Sensitivity**; Laurence Mayrand Provencher¹; Vinicio Vasquez¹; Milton Furtado¹; Anahita Keyhani¹; ¹Altasciences, Laval, QC, Canada
- MP 671 **Screening and Quantification of Unapproved Dietary Supplements using Liquid Chromatography with Quadrupole-Orbitrap Mass Spectrometry**; Flavia Morales-Garcia¹; Douglas M. Monroe¹; Judith Hillegas¹; Tracy A. Majkol¹; Joan M. Nandrea¹; Fenhong Song²; Aref El-Demerdash¹; ¹FDA, Lenexa, KS; ²FDA, Rockville, MD
- MP 672 **Quantitative Analysis of Antiarrhythmic Drugs in Human Plasma Using a High Performance Triple Quadrupole Mass Spectrometer**; Keeley Murphy¹; Claudia Martins²; Jonathan Josephs²; ¹Thermo Fisher Scientific, San Jose, CA; ²ThermoFisher, San Jose, CA
- MP 673 **Simultaneous Analysis of Emtricitabine, Tenofovir, and Efavirenz in Mouse Plasma, Amniotic Fluid, and Fetus Homogenate by UPLC-MS/MS**; Brenda L. Fletcher¹; Melanie A. Rehder Silinski¹; Reshan A. Fernando¹; Veronica G. Robinson²; Suramya Waidyanatha²; ¹RTI International, Research Triangle Park, NC; ²Division of National Toxicology Program, NIEHS, Research Triangle Park, NC
- MP 674 **Tenofovir and Emtricitabine Quantification in Cervicovaginal Fluid: Collection Device Considerations in Support of Clinical Trials**; Teresa L. Parsons¹; Lauren A. Sesecko¹; Mark A. Marzinko¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
- MP 675 **Resin-Coated Proppant Analysis for Formaldehyde Content by GC-MS Headspace, GC-VUV, and HPLC**; Jamie Schenk¹; Doug D. Carlton Jr.^{1,2}; Jonathan Smuts³; Ty Hanna⁴; Danny Durham⁴; Kevin A. Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²CLEAR, Arlington, TX; ³VUV Analytics, Inc., Austin, TX; ⁴Apache Corporation, Houston, TX
- MP 676 **Method Conversion Tool between Instruments for Huge-Multiple MRM Transitions in LC-MS/MS Adopting the Conversion Factor of Collision Energy Voltage**; Akane Yamamoto¹; Kazutaka Ikeda²; Yoshiki Tainaka¹; Jun Watanabe¹; ¹Shimadzu Corporation, Kyoto, Japan; ²RIKEN Center for Integrative Medical Sciences, Yokohama, Japan
- MP 677 **Highly Sensitive Simultaneous Quantitative Analysis of Estrone and Equilin from Plasma using LC/MS/MS**; Ashutosh Shelar¹; Shailendra Rane¹; Shailesh Damale¹; Rashmi Kochhar¹; Purushottam Sutar¹; Deepti Bhandarkar¹; Anant Lohar¹; Ajit Datar¹; Pratap Rasam¹; Jitendra Kelkar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 678 **Analysis of Glucosamine in Functional Foods by LC-MS/MS**; Shin Yong Woon; Ministry of Food & drug Safety, Cheongju, Chungcheongbuk-do
- MP 679 **LC/MS/MS Analysis of Fentanyl and Related Analogs Using Biocompatible Solid Phase Microextraction**; Candace Price¹; Craig Aurand¹; Sara Smith¹; Emily Barrey¹; ¹MilliporeSigma, Bellefonte, PA
- MP 680 **Validation of a LC-MS/MS Method for Quantification of Digoxin in Triton X-100 Fortified Human Urine**; Damon Papac¹; Brian M Murray¹; James Vannicola¹; Eugene F Miller¹; Debra J Beck¹; Kristine Wagner-Carusol¹; ¹Icon Plc, Whitesboro, NY
- MP 681 **Bionalysis of Fluticasone Propionate in Rabbit Plasma and Nasal/Sinus Tissue using Sensitive LC/MS/MS Methods**; Patrick Lin¹; Bih-Hsiung Hsu¹; ¹PHARMout Lab, Sunnyvale, CA



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- MP 682 **Simultaneous Determination of Dihydrotestosterone and Its Metabolites in Mouse Sera by LC-MS/MS with Chemical Derivatization**; [Shashank Gorityala](#)¹; Shuming Yang²; Monica M Montano³; Yan Xu^{1,2}; ¹*Department of Chemistry, Cleveland State University, Cleveland, OH*; ²*Case Comprehensive Cancer Center, Case Western Reserve University, Cleveland, OH*; ³*Department of Pharmacology, Case Western Reserve University, Cleveland, OH*
- MP 683 **Methods for the Determination of Drugs of Abuse in Oral Fluids Using an Automated Sample Preparation and uHPLC-MS/MS**; [Larry M Mallis](#)¹; Brenna Espelien¹; Erich Valenzuela¹; Benjamin Moeller¹; Yongquan Lai¹; Jacob Jantzi¹; Ryan Sheeler¹; Philip Kuehl¹; Jacob McDonald¹; ¹*Lovelace Biomedical, Albuquerque, NM*
- MP 684 **Capture Efficiency and Separation Performance of Dynamic pH Junction Focusing with Two On-Column Electrolyte Configurations in Capillary Electrophoresis Mass Spectrometry**; [Lingyu Wang](#)¹; David D. Y. Chen¹; ¹*University of British Columbia, Vancouver, BC, Canada*
- MP 685 **A High Throughput UPLC-MS/MS Method for the Simultaneous Determination of Pravastatin and Rosuvastatin in Human Urine**; [Feng-Ming James Chang](#)¹; Yuan-Shek Chen¹; T. Ben Hsu¹; ¹*QPS, LLC, Newark, DE*
- MP 686 **Development of Combined LC-MS/MS Analysis for Citric Acid Cycle Intermediates, Acylcarnitines and Amino Acids**; [Rohan R Shah](#)¹; Alisha House¹; Erica M Fatica¹; Yana Slanders¹; ¹*Cleveland State University, Department of Chemistry, Cleveland, OH*
- MP 687 **Quantitation of 25OH Vitamin D2/D3 in Serum by a New SLE Method Coupled with LC-MS/MS**; [Guotao Lu](#)¹; Warren Chen¹; Wan Wang²; Suzi Qin²; Lei Yin²; ¹*Bonna-Agela Technologies, Wilmington, DE*; ²*Bonna-agela Technologies Inc., Tianjin, China*
- MP 688 **Analysis of GSK525762 and Its Major Oxidative Metabolites in Human Plasma using Liquid Chromatography with Tandem Mass Spectrometric Detection**; [Zhilong Gong](#)¹; Chineta Barksdale²; Kelly Connelly³; Omobola Oladipupo²; Eric Thomas²; ¹*Covance Bioanalytical Svc, Indianapolis, IN*; ²*Covance, Indianapolis, IN*; ³*GlaxoSmithKline, Ware, UK*
- MP 689 **A Special Preparation to Improve Phosphocholine Determination in Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; [jing Tan](#)¹; Chunyan Zhang¹; Jason Gek Leong Neo¹; Tania Setiawati¹; ¹*Abbott Nutrition, Singapore*

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- MP 690 **Web-Based Implementation of Kinase-Substrate Enrichment Analysis (KSEA) for Phosphoproteomics-Derived Kinase Activity Inference**; [Danica Wiredja](#)^{1,2}; Mehmet Koyutürk^{1,3}; Mark R. Chance^{1,2}; ¹*Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH*; ²*Department of Nutrition, Case Western Reserve University, Cleveland, OH*; ³*Department of Electrical Engineering and Computer Science, Case Western Reserve University, Cleveland, OH*
- MP 691 **Protein Expressional Changes of Pseudomonas aeruginosa in Lactate-Supplemented Media**; [Yeni P. Yung](#)¹; S Lee McGill¹; Stephanie M. Cologna¹; Hui Chen¹; Ross P. Carlson²; Luke Hanley¹; ¹*University of Illinois at Chicago, Chicago, IL*; ²*Montana State University, Bozeman, MT*
- MP 692 **Quantitative Proteomics of the Host-Pathogen Interplay during Salmonella Typhimurium Infection**; [Jennifer Geddes-McAlister](#)¹; Felix Meissner¹; ¹*Max Planck Institute of Biochemistry, Martinsried, Germany*
- MP 693 **Proteogenomic Landscape of Squamous Cell Lung Cancer**; [Paul A Stewart](#)¹; Robbert JC Slebos¹; Eric A Welsh¹; Ling Cen¹; Yonghong Zhang¹; Zhihua Chen¹; Chia-

- Ho Cheng¹; Fredrik Pettersson¹; Anders Berglund¹; Guolin Zhang¹; Bin Fang¹; Victoria Izumi¹; Sean Yoder¹; Katherine Fellows¹; Yian Ann Chen¹; Jamie K Teer¹; Steven A Eschrich¹; John M Koomen¹; Eric B Haura¹; ¹*Moffitt Cancer Center, Tampa, FL*
- MP 694 **Pharmacoproteomic Characterisation of Human Colon and rectal Cancer**; [Martin Frejino](#)^{1,2}; Riccardo Zenezini Chiozzi^{1,3}; Mathias Wilhelm¹; Heiner Koch^{1,4,5,6}; Runsheng Zheng¹; Susan Klaeger^{1,5,6}; Benjamin Ruprecht^{1,7}; Chen Meng¹; Karl Kramer¹; Anna Jarzab¹; Stephanie Heinzlmeir^{1,5,6}; Elaine Johnstone²; Enric Domingo^{2,8}; David Kerr⁹; Moritz Jesinghaus¹⁰; Julia Slotta-Huspenina¹⁰; Wilko Weichert¹⁰; Stefan Knapp¹¹; Stephan M Feller^{12,13}; Bernhard Kuster^{1,5,7,14}; ¹*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*; ²*Department of Oncology, University of Oxford, Oxford, UK*; ³*University of Rome, La Sapienza, Rome, Italy*; ⁴*Max Planck Institute of Biochemistry, Martinsried, Germany*; ⁵*German Cancer Consortium (DKTK), Munich, Germany*; ⁶*German Cancer Research Center (DKFZ), Heidelberg, Germany*; ⁷*Center for Integrated Protein Science Munich, Freising, Germany*; ⁸*Wellcome Trust Centre for Human Genetics, University of Oxford, Oxford, UK*; ⁹*Nuffield Division of Clinical Laboratory Sciences, University of Oxford, Oxford, UK*; ¹⁰*Institute of Pathology, Technical University of Munich, Munich, Germany*; ¹¹*Institute of Pharmaceutical Chemistry, Goethe University, Frankfurt am Main, Germany*; ¹²*Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, UK*; ¹³*Institute of Molecular Medicine, Martin-Luther-University, Halle (Saale), Germany*; ¹⁴*Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*
- MP 695 **Integration of Metabolomics Data with Kinetic Models for Dynamic Flux Analysis and the Inference of Biochemical Mechanisms**; [Zhen Qi](#)¹; ¹*Lexington, KY*
- MP 696 **12-week Aerobic, Resistance, and Combined Training Shows Posttranslational Regulation of Skeletal Muscle in Younger and Older Adults**; [Matthew M. Robinson](#)¹; Surendra Dasari²; Adam R. Konopka³; Matthew L. Johnson⁴; S. Manjunatha²; Raul R. Esponada⁵; Rickey E. Carter²; Ian R. Lanza²; K. Sreekumaran Nair²; ¹*Oregon State University, Corvallis, OR*; ²*Mayo Clinic, Rochester, MN*; ³*Colorado State University, Fort Collins, CO*; ⁴*Dexcom, San Diego, CA*; ⁵*Sanford Health, Fargo, ND*
- MP 697 **Longitudinal Metaproteomics Analysis of Premature Infant Intestinal Microbiota Reveals Early-Life Microbial and Host Metabolic Functions**; [Weili Xiong](#)¹; Chris T Brown²; Matthew B Rogers³; Michael J Morowitz³; Jillian F Banfield²; Robert L Hettich¹; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*; ²*Department of Earth and Planetary Science, UC, Berkeley, CA*; ³*School of Medicine, University of Pittsburgh, Pittsburgh, PA*
- MP 698 **Infrared Laser Ablation Sample Transfer with Conserved Biological Function**; Kelin Wang¹; Matthew D. Baldone¹; Fabrizio Donnarumma¹; [Kermit K. Murray](#)¹; ¹*Louisiana State University, Baton Rouge, LA*
- MP 699 **Inferring Metabolic Function across Wildly Variable Gut Metaproteomes Derived from Crohn's Disease Patients Post Resection Surgery**; [J. Alfredo Blakeley-Ruiz](#)¹; Alison R Erickson²; Weili Xiong³; Claire M. Fraser⁴; Robert L Hettich³; ¹*University of Tennessee, Knoxville, TN*; ²*Harvard Medical School, Boston, MA*; ³*Oak Ridge National Laboratory, Oak Ridge, TN*; ⁴*University of Maryland School of Medicine, Baltimore, MD*
- MP 700 **ProHits-viz: A Suite of Web-Tools for Visualizing Interaction Proteomics Data**; James D R Knight¹; Hyungwon Choi²; Brian Raught³; Alexey I Nesvizhskii⁴; [Anne-Claude Gingras](#)^{1,5}; ¹*Lunenfeld-Tanenbaum Research Institute, Toronto, Ontario*; ²*National University of Singapore, Singapore, Singapore*; ³*Princess Margaret Cancer Centre, Toronto, ON, Canada*; ⁴*Department of Pathology, University*



- of Michigan, Ann Arbor, MI; ⁵Department of Molecular Genetics, University of Toronto, Toronto, ON, Canada
- MP 701 **Diagnosis of Ecosystem Adaptive Responses by Analysis of Hundreds of Peptide Biomarkers in the North Atlantic Ocean using Targeted Metaproteomics;** Mak Saito¹; Matthew McIlvin¹; Dawn Moran¹; Luis Valentin¹; Romain Huguet²; Shannon Eliuk²; Graeme McAlister²; Rod Johnson³; ¹Woods Hole Oceanographic Inst., Woods Hole, MA; ²ThermoFisher, San Jose, CA; ³Bermuda Institute of Ocean Sciences, St. George's, Bermuda
- MP 702 **An Integrated Omics Approach to Characterize Complex Microbial Phenotype Behavior: Characterizing Bacterial Swarming;** Robert Hettich¹; Richard J Giannone¹; James Elkins¹; Jenny Morrell-Falvey¹; Abigail Tester²; Shawn R Campagna²; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN
- MP 703 **Leveraging Transcriptomic and Phosphoproteomic Data of Perturbed MCF10A Cells to Identify Downstream PTEN Events of Breast Cancer;** Chenwei Lin¹; Richard Ivey¹; Jacob J Kennedy¹; Ping Yan¹; Jeffery R. Whiteaker¹; Julia Voytovich¹; Travis Lorentzen¹; Regine Schoenherr¹; Amanda G. Paulovich¹; Pei Wang²; ¹Fred Hutchinson CRC, Seattle, WA; ²ICahn Institute for Genomics and Multiscale Biology, New York, NY
- MP 704 **A Systems Toxicology Approach to Predict Disease-Like Phenotypes in Human Lung Tissue Models;** Joseph Caruso¹; Paul Stemmer¹; ¹Institute of Environmental Health Sciences, Wayne State University, Detroit, MI
- MP 705 **A Label-Free Informatics Framework for Automated Top-Down Proteoform Relationship Determination and Protein Identification across Multidimensional Chromatographic Space;** Steven Patrie¹; Casey E Wing¹; John R Corbett¹; William S Phipps¹; Daniel A Plymire¹; ¹UT Southwestern Med. Center, Dallas, TX
- MP 706 **Mass-Spectrometry of Single Mammalian Cells Quantifies Proteome Heterogeneity during Cell Differentiation;** Bogdan Budnik¹; Ezra Levy²; Harrison Specht²; Nikolai Slavov³; ¹Harvard University, Cambridge, MA; ²Northeastern University, Boston, MA; ³Northeastern University, Boston, MA
- TOXICOLOGY**
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- MP 707 **An Ultrafast, Dilute and Shoot-Flow Injection/ MRM method for Quantification of Phenobarbital and Ethyl-D-Glucuronide (EtG) in Urine;** Ravali Alagandula; Cleveland State University, Cleveland, OH
- MP 708 **Determination of cis-Permethrin, Trans-Permethrin in Rat Plasma and Brain using Gas Chromatography–Negative Chemical Ionization Mass Spectrometry;** Shirin Hooshfar¹; Darren Gullick¹; Michael Linzey¹; Tanzir Mortuza¹; James V. Bruckner¹; Catherine A. White¹; Michael G. Bartlett¹; ¹Department of Pharmaceutical and Biomedical Sciences, College of Pharmacy, The University of Georgia, Athens, GA
- MP 709 **Development of multi-Residue LC-MS/MS Method for Determination of Mycotoxins in Animal Feed;** Renat Selimov¹; Pavel Metalnikov²; Alexander Komarov²; ¹VGNKI, Moscow, Russia; ²VGNKI, Moscow, Moscow
- MP 710 **Development of an Analytical Method for 2,2'-Dimorpholinodiethyl Ether (DMDEE), in Rat Plasma, Amniotic Fluid, and Fetus Homogenate by UPLC-MS/MS;** Teruyo Uenoyama¹; Melanie A. Rehder Silinski¹; Reshan A. Fernando¹; Veronica G. Robinson²; Georgia K. Roberts²; Suramya Waidyanatha²; ¹RTI International, Research Triangle Park, NC; ²Division of National Toxicology Program, NIEHS, Research Triangle Park, NC
- MP 711 **Combined Screening and Quantitative Confirmation of 110 Drugs in Urine by LDTD-MS/MS Using a Generic SPE Procedure;** John D. Laycock¹; Serge Auger²; Pierre Picard²; Philip Dimson¹; Karsten Liegmann¹; David Hall¹; Jean Lacoursiere²; ¹Tecan-SP, Baldwin Park, CA; ²Phytronix Technologies, Québec, QC, Canada
- MP 712 **Point-of-Care Identification of Ingested Household Pesticides in Gastric Lavage Content by Laser Desorption-Electrospray Ionization Mass Spectrometry in the Emergency Department;** Chi-Wei Lee¹; Hung Su²; Yang-Kuang Pan²; Jentaie Shiea²; ¹Kaohsiung Medical University, Kaohsiung, Taiwan; ²National Sun Yat-Sen University, Kaohsiung, Taiwan
- MP 713 **Toxicological Screening for over 1000 Compounds in an MRM Based Acquisition for Library ID in Whole Blood Samples;** Alan Barnes¹; Tiphaine Robin²; Sylvain Dulaurent²; Souleiman Elbalkhi²; Stéphane Moreau³; Neil Loftus¹; Pierre Marquet²; Franck Saint-Marcoux²; ¹Shimadzu Corporation, Manchester, UK; ²CHU Limoges, Limoges, France; ³Shimadzu Europa GmbH, Duisburg, Germany
- MP 714 **Automatic, Simultaneous and Rapid Analysis of 22 Drugs of Abuse in Saliva by on Line SPE and UHPLC-MS/MS;** Toïnon Doriane¹; Jaffuel Aurore²; Huteau Alban²; ¹Shimadzu, Noisiel; ²Shimadzu France, Paris, France
- MP 715 **Analysis of the Chemical Warfare Agent VX Isomers in Guinea Pig Blood Following an IV Exposure Utilizing Normal Phase LC-MS/MS;** Christopher E Byers¹; Michael W Busch²; Paul S Demond²; Linnzi K. Wright¹; Ronald A Evans¹; ¹US Army ECBC, Aberdeen Proving Ground, MD; ²Excet, Inc., Springfield, VA
- MP 716 **Analysis of Genital Abnormalities Induced by Fetal Exposure to Endocrine Disrupting Chemicals via Shotgun Proteomics;** Tara Nash¹; Ciro M Amato²; Josua Mogus²; Krista McCoy²; Michael S Bereman¹; ¹North Carolina State University, Raleigh, NC; ²East Carolina University, Greenville, NC
- MP 717 **Comparison of Genetic and Environmental Mechanisms of Motor Neuron Death by Contemporary Proteomics;** Joshua Beri¹; Tara Nash¹; Micheal Bereman¹; ¹North Carolina State University, Raleigh, NC
- MP 718 **Data Dependent or Data Independent Acquisition: Evaluation of SWATH for Clinical and Forensic Drug Screening;** Kara L. Lynch¹; Jeffrey D. Whitman¹; ¹University of California, San Francisco, San Francisco, CA
- MP 719 **Elucidation of the Epiproteomic Landscape at the Arsenic Response Locus in S. cerevisiae by CRISPR-ChAP-MS;** Kirk L West¹; Zachary J Waldrip²; Stephanie Byrum²; Ricky D Edmondson²; Sam G Mackintosh²; Sean D Taverna³; Alan J Tackett²; ¹Univ. of Arkansas for Medical Sciences, Little Rock, AR; ²UAMS, Little Rock, AR; ³Johns Hopkins School of Medicine, Baltimore, MD
- MP 720 **Investigation of Saliva as an Alternative Matrix for General Unknown Screening of Drugs of Abuse and Medication;** Michael Boettcher¹; Markus Meyer²; ¹MVZ Labor Dessau GmbH, Dessau-Rosslau, Germany; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 721 **Quantitative Clinical Toxicological Screening Comparing Library ID from Product Ion Scan MS/MS to MRM Spectrum Mode ID;** Alan Barnes¹; Tiphaine Robin²; Sylvain Dulaurent²; Souleiman Elbalkhi²; Neil Loftus¹; Pierre Marquet²; Franck Saint-Marcoux²; ¹Shimadzu Corporation, Manchester, UK; ²CHU Limoges, Limoges, France



TUESDAY POSTERS

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Odd-numbered posters present 10:30 am – 1:00 pm
Even-numbered posters present 12:00 – 2:30 pm
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- TP 001 ***in situ* Mass Spectrometry for Chemical Identification of Live Cells with Milliseconds Level Ultrafast Electrophoresis**; Guangming Huang¹; Hongying Zhu¹; Gongyu Li¹; ¹USTC, Hefei, Anhui
- TP 002 **Screening of Skin Lightening Products for the Corticosteroid Clobetasol Propionate using Direct Analysis in Real Time (DART) and Mass Detection**; Marian Twohig¹; Oliver Burt²; Chris Stumpf¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- TP 003 **Ultra-fast Screening of Pesticides in Foods and Agricultural Products with Desorption Corona Beam Ionization (DCBI) Tandem Mass Spectrometry**; Jing Dong¹; Satoshi Yamaki²; Yuki Hashi³; Naoki Hamada¹; ¹Shimadzu China, Beijing, China; ²Shimadzu Corporation, Kanagawa, Japan; ³Shimadzu China, Shanghai, China
- TP 004 **Open Probe Fast GC-MS for Medical Diagnostics and Drug Pills Real Time Analysis**; Uri Keshet¹; Ramesh Bokka¹; Alexander B. Fialkov¹; Tal Alon¹; Aviv Amirav¹; ¹Tel Aviv University, Tel Aviv, Israel
- TP 005 **A Novel Universal and Direct SPME-MS Interface Based on Capillary APPI for Simultaneous Quantitation of Polar and Nonpolar Compounds**; Mario Francesco Mirabelli¹; Renato Zenobi¹; ¹ETH Zurich, Zurich, CH
- TP 006 **Cleavable Isobaric Peptides as Mass Reporters for**

- Mass Spectrometry-based Immunoassays**; Tatiana Vélez-Burgos¹; Jay Kim¹; Yosef Maher¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- TP 007 **Detection and Quantification of Atomic Ions with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry**; Garett M. MacLean¹; Jacob T. Shelley¹; ¹Rensselaer Polytechnic Institute, Troy, New York
- TP 008 **Extractive Atmospheric Pressure Photoionization (EAPPI) Mass Spectrometry: Rapid Analysis of Chemicals in Complex Matrices**; chengyuan liu¹; Yang Pan¹; ¹University of Science and Technology of China, Hefei, China
- TP 009 **Molecular Characterization of Exhaust Particulate Matters Using Internal Extractive Electrospray Ionization Mass Spectrometry**; Hua Zhang^{1,2}; Yi Li²; Liang Zhu²; Huanwen Chen²; ¹State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China; ²East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China
- TP 010 **Rapid Classification of Medulloblastoma Subgroups for Optimal Treatment Planning Using a Hand Held Cold Laser Ablation Mass Spectrometry Probe**; Michael Woolman¹; Jing Zou¹; Megan Wu²; Semra Isik²; Claudia M Kuzan-Fischer²; Isabelle Ferry²; Sunit Das²; Michael D Taylor²; James T Rutka²; Howard Ginsberg¹; Arash Zarrine-Afsar³; ¹University of Toronto, Toronto, ON; ²Hospital for Sick Children, Toronto, Ontario; ³Toronto, ON
- TP 011 **Rapid Molecular Analysis and Comparison of Canine, Feline and Human Tumour Samples with REIMS; Metastasis based Identification of Primary Tumour**; Julia Balog^{1,2}; Richard Schaffer¹; Steven Derek Pringle^{2,3}; Zoltan Takats²; ¹Waters Research Center, Budapest; ²Imperial College London, London; ³Waters Corporation, Manchester
- TP 012 **Thermal Desorption Combined with Flame Atmospheric Pressure Chemical Ionization Mass Spectrometry to Rapidly Determine Chemical Compounds**; Hung Su¹; Shih-Hsi Chen¹; Sy-Chyi Cheng¹; Jentaie Shiea¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan
- TP 013 **Utilizing Solid Phase Extraction Technologies to Facilitate DART-based High-Throughput Ambient Ionization-MS Analysis of Biological Samples**; Brian D. Musselman¹; Fredrick Li¹; Joseph Tice¹; ¹IonSense, Inc., Saugus, MA
- TP 014 **A Comparative Study of Nitrogen Versus Helium Direct Analysis in Real Time Mass Spectrometry for the Analysis of Polar Compounds**; Liguang Song¹; Wei Chean Chuah¹; Edward Remsen²; John E Bartmess³; ¹Western Illinois University, Macomb, IL; ²Bradley University, Peoria, IL; ³University of Tennessee, Knoxville, TN
- TP 015 **Analysis of Degraded Polybutylene Terephthalate (PBT) Products by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**; Chikako Takei¹; Yasuyuki Semba¹; Kenichi Yoshizawa¹; ¹BioChromato, Inc., Fujisawa, Japan
- TP 016 **Analysis of Macrolides Antibiotics by Direct Analysis in Real-Time Mass Spectrometry with Glycerin as Dopant**; Qing Yang¹; Jiyan Guo¹; Bin Xu²; Weihong Zhang²; Xiaokun Duan²; Charles C. Liu²; ¹Department of Quality Inspection, New Hope Liuhe Co., Ltd, Qingdao, China; ²ASPEC Technologies LTD, Beijing, China
- TP 017 **Analysis of Tea Aroma by Direct Analysis in Real-Time Mass Spectrometry**; Li Zhang¹; Bin Xu²; Xiaokun Duan²; Charles C. Liu²; ¹Suzhou Vocational University, Suzhou, China; ²ASPEC Technologies LTD, Beijing, China
- TP 018 **Analysis of Weakly Interacting Dicopper Formamidinate Complexes by Direct Analysis in Real Time (DART) Mass Spectrometry**; Michael Pastor¹; O. David Sparkman¹; Qinliang Zhao¹; ¹University of the Pacific,



- Stockton, California
- TP 019 **Chemotaxonomy of *Astyanax* and *Drosophila* by DART-MS Analysis of fatty acids and Ozonolysis-Derived Fatty Acyl Fragments;** Joanne Y. Yew¹; Masato Yoshizawa²; Robert B. Cody³; ¹Pacific Biosciences Research Center, University of Hawaii at Manoa, Honolulu, HI; ²Department of Biology, University of Hawaii at Manoa, Honolulu, HI; ³JEOL USA Inc., Peabody, MA
- TP 020 **Comparison of Portable near-IR and Laboratory mid-IR Sources for Laser Ablation Atmospheric Pressure Photoionization MS;** Raveendra C. Wickramasinghe¹; Yeni P. Yung¹; Anu Vaikkinen²; Tiina J. Kaupila²; Luke Hanley¹; ¹University of Illinois at Chicago, Chicago, IL; ²University of Helsinki, Helsinki, Finland
- TP 021 **Dark Discharge Assisted Direct Analysis in Real Time Ionization using Argon;** Motoshi Sakakura¹; Teruhisa Shiota¹; Mitsuo Takayama²; Kanako Sekimoto^{2,3}; ¹AMR Inc., Meguro-ku, Japan; ²Yokohama City Univ., Yokohama, Japan; ³NOAA Earth System Research Laboratory, Boulder, CO
- TP 022 **MS/MS Applications of the iKnife in Breast Surgery: Towards Triple-Quadrupole Based Real-Time Tissue Identification;** Zsolt Bodai¹; Edward St John¹; Emma White¹; April Covington¹; James McKenzie¹; Francesca Rosini¹; Hui-Yu Ho¹; Julia Balog²; Daniel Leff¹; Zoltan Takats¹; ¹Imperial College London, London; ²Waters Research Center, Budapest
- TP 023 **Rapid Detection of Explosives using Thermal Desorption DART-MS and Reverse Library Search;** Frederick Li¹; Joseph Tice¹; Stephen Shrader²; Brian Musselman¹; ¹IonSense Inc., Saugus, MA; ²Shrader Software Solutions, Grosse Pointe Park, MI
- TP 024 **Rapid Screening of Explosives in Ambient Environment by Aerodynamic Assisted Thermo Desorption Mass Spectrometry;** Jianli Liu¹; Qiang Zhao¹; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, China
- TP 025 **Real-Time Organic Aerosol Analysis via Vacuum-assisted Plasma Ionization (VaPI) Ion Mobility-Mass Spectrometry;** Sandra L. Blair¹; Stephen C. Zambrycki¹; Anyin Li¹; Masayuki Takeuchi¹; Charles L. Liotta¹; Nga L. Ng¹; Facundo M. Fernández¹; ¹Georgia Institute of Technology, Atlanta, GA
- ANTIBODIES & ANTIBODY DRUG CONJUGATES II**
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- TP 026 **Elimination of ADE-induced Dengue Virus Infection by a Novel Reagent DCAF;** Shan Feng; Tsinghua University, Beijing, Beijing; University of Notre Dame, Notre Dame, IN
- TP 027 **Investigating Product Quality of HIV Monoclonal Antibody by LC-MS Analysis;** Vera B. Ivleva¹; Nicole A. Schneck¹; Q. Paula Lei¹; K. C. Cheng¹; ¹NIH/NIAID/VPPL, Gaithersburg, MD
- TP 028 **Evaluation of Protein Aggregation in Biopharmaceutical using Chemical Cross-linking MS and Quantitative Laser diffraction;** Yuza Yamazaki¹; Kenji Saito²; Hiroki Maeda¹; Yuji Shoya²; Masayoshi Toyoura²; ¹Shimadzu Corporation, Kyoto, Japan; ²Biomedical R&D Department, Pharma Foods International, Japan
- TP 029 **Factors Affecting Spectral Quality of Monoclonal Antibodies from Time-of-Flight Mass Spectrometers;** Jeff Brown¹; Jonathan Williams¹; Emmy Hoyes¹; Dale Cooper-Shepherd¹; Francesco Lanucara¹; Laetitia Denbigh¹; Michael Morris¹; ¹Waters Corporation, Wilmslow, UK
- TP 030 **Characterization of a Cysteine-conjugated ADC on a Hybrid Quadrupole-Orbitrap Mass Spectrometer;** Xiaoxi Zhang¹; Jun Lin²; ¹ThermoFisher Scientific, Shanghai, China; ²Genor Biopharma Co., Ltd., Shanghai, China
- TP 031 **Characterizing and Quantitating Therapeutic Antibody and Drug Conjugate Biotransformation using High Throughput On-Tip Affinity Capture Mass Spectrometry;** John C. Tran¹; Ke Sherry Li²; Jianyong Wang²; Phillip Y Chu²; Aimee Fourie²; Robert Tchelepi²; Katherine R Kozak²; Yichin Liu²; ¹Genentech, South San Francisco, CA; ²Genentech, Inc, South San Francisco, CA
- TP 032 **Qualitative Analysis of Antibody-Drug Conjugates (ADCs): An Experimental Evaluation of Common Analytical Techniques for Direct Comparison;** Malin Källsten^{1,2}; Rafael Hartmann^{1,2}; Konstantin Artemenko¹; Fredrik Lehmann²; Jonas Bergquist¹; ¹Uppsala University, Uppsala, Sweden; ²Recipharm OT Chemistry AB, Uppsala, Sweden
- TP 033 **Understanding the Limits of Quantitation for Intact Proteins using Microfluidic LC-MS;** Gregory Roman¹; James Murphy¹; ¹Waters Corp, Milford, MA
- TP 034 **Comprehensive Characterization on Monoclonal Antibody using a Newly Developed Q-TOF/MS Instrument;** David Wong¹; Jing Chen²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Madison, WI
- TP 035 **Gas-phase rearrangement by CID of Calicheamicin-based LP with Cleavable Linker Containing Aminobenzylcarbamate Group;** Xidong Feng¹; Dahui Zhou¹; Kenneth Dirico¹; Russell Dushin¹; Chakrapani Subramanyam¹; Christopher J O'Donnell¹; ¹Pfizer, Groton, CT
- TP 036 **Development of Native and Denaturing LC-MS Methods for Characterization of Cysteine-Linked Antibody Drug Conjugates Using a Non-Toxic Mimic;** Kevin Ray¹; Nicolas Caffarelli¹; Gordon Nicol¹; Ben Cutak¹; Brian Gau¹; Jeff Turner¹; ¹MilliporeSigma, St. Louis, MO
- TP 037 **Hybrid-MS Analyses of IgG1 Antibodies: Confirmation of Conformation;** Rosie Upton¹; Kamila J Pacholarz¹; Lukasz Migas¹; Amy Campbell²; Perdita E Barran¹; David Firth³; ¹University of Manchester, Manchester, UK; ²University of Liverpool, Liverpool, Merseyside; ³Covance Laboratories Ltd., Harrogate, UK
- TP 038 **Native Ion Mobility Mass Spectrometry for the Characterization of Biotherapeutics;** Dale A. Cooper-Shepherd¹; Jakub Ujma¹; Kevin Giles¹; Laetitia F. Denbigh¹; Nick Tomczyk¹; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- TP 039 **Insights from Native Mass Spectrometry Approaches for Top- and Middle- Level Characterization of Site-Specific Antibody-Drug Conjugates;** Thomas Botzanowski¹; Stephane Erb¹; Oscar Hernandez Alba¹; Anthony Ekhkirch¹; Olivier Colas²; Elsa Wagner-Rousset²; David Rabuka³; Penelope Drake³; Alain Beck²; Sarah Cianferani¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; ²Centre d'Immunologie Pierre-Fabre, Saint-Julien-en-Genevois, France; ³Catalent Biologics West, Emeryville, CA
- TP 040 **Characterizing Trastuzumab-Drug Conjugates by High Resolution Native Mass Spectrometry, Ion Mobility, and Molecular Dynamics Simulations;** Liuqing Shi¹; Bernadette V. Marquez-Nostra²; Suzanne E. Lapi³; Weidong Cui⁴; Michael L. Gross¹; ¹Washington University, St Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³University of Alabama at Birmingham, Birmingham, AL; ⁴Washington University, St. Louis, MO
- TP 041 **Higher Order Structural Analysis of Biotherapeutics Exposed to Sample Handling Stress Conditions;** Richard A Kerr¹; Hongping Ye¹; ¹FDA Department of Pharmaceutical Analysis, St Louis, MO
- TP 042 **Intact Mass Analysis and DAR Calculation for Antibody-Drug Conjugates;** Marshall W. Bern¹; Yong J. Kil¹; Eric Carlson¹; K. Ilker Sen¹; St John Skilton¹; Michael Peddicord²; Wei Ding²; ¹Protein Metrics Inc., San Carlos, CA; ²Bristol-Myers Squibb, New Brunswick, NJ
- TP 043 **Evaluation of an ADC's DAR in Rat Serum by Affinity**



TUESDAY POSTERS

- Capture and Mass Spectrometry;** Maria Christina Malinao¹; Cody A Warhurst¹; Julien Dugal-Tessier¹; Josh T. Snyder¹; Brian A Mendelsohn¹; ¹*Agensys, Inc., Santa Monica, CA*
- TP 044 **How to Tailor Holistic Analytical Solutions for Therapeutic Bioconjugates to Reveal Previously Unknown Conjugatable Modifications;** Wesley Zmolek¹; Qiuting Hong¹; William E Haskins¹; ¹*Redwood Bioscience (Catalent Biologics-West), Emeryville, CA*
- TP 045 **A Mass Spectrometric Method for Readily Identifying Peptides Modified with vcMMAE in Antibody-Drug Conjugate Enzyme Digests;** Ioannis A Papayannopoulos¹; Shannon Renn-Bingham¹; Jarrod M Womble¹; ¹*Celldex Therapeutics, Inc., Fall River, MA*
- TP 046 **Analysis of Monoclonal Antibodies in Human Serum for Monoclonal Gammopathy Diagnosis by 21 Tesla FT-ICR Top-Down and Middle-Down MS/MS;** Lidong He¹; Lissa Anderson²; David R. Barnidge³; David L. Murray³; Christopher L Hendrickson^{1,2}; Alan G. Marshall^{1,2}; ¹*Florida State University, Tallahassee, Florida*; ²*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*; ³*Mayo Clinic, Rochester, MN*
- TP 047 **Kinetics of Intracellular Dolastatin Accumulation in EGFR Expressing Cell Lines after Antibody-drug Conjugate Dosing;** Ken Durbin; *AbbVie, North Chicago, IL*
- TP 048 **De-conjugation Coupled with LC-MS for Investigating the Stability of Small Molecule Drugs in Antibody-Drug Conjugates;** Tao Chen¹; Dian Su¹; Jason Gruenhagen¹; Yi Li¹; Peter Yehl¹; Nik Chetwyn¹; Colin Medley¹; ¹*Genentech, Inc., South San Francisco, CA*
- TP 049 **Application of ETD to the Characterization of ADC Product Attributes That Are Challenging to the Traditional Approach;** Zhiqi Hao¹; Qiuting Hong^{2,3}; Michael Kim¹; Diana Liu¹; William Haskins^{1,3}; Yan Chen¹; ¹*Genentech, Inc, South San Francisco, CA*; ²*Eurofins Lancaster Laboratories, Inc., Lancaster, PA*; ³*Catalent Pharma Solutions, Emeryville, CA*
- TP 050 **Characterization of a Degradation Product of an IgG1 Monoclonal Antibody by Tandem Mass Spectrometry and Other Biophysical Techniques;** Ekaterina G. Deyanova¹; Yun Wang²; Yuan Cheng²; Jun Dai²; Brent Meengs³; Jason Chen²; Jonathan Wert³; Yingru Zhang²; Olafur Gudmundsson²; Susan Julien³; Guodong Chen²; ¹*Bristol-Myers Squibb, Princeton, NJ*; ²*Bristol-Myers Squibb, Princeton, NJ*; ³*Bristol-Myers Squibb, Seattle, WA*
- TP 051 **A Direct Comparison of Top-Down and Bottom-Up HDX-MS for Antibody Characterization;** Jingxi Pan^{1,2}; Suping Zhang³; Christoph H. Borchers^{1,4}; ¹*University of Victoria - Genome BC Proteomics Centre, Victoria, BC*; ²*Division of Medical Sciences, University of Victoria, Victoria, BC*; ³*MRM Proteomics, Victoria, BC*; ⁴*Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC*
- TP 052 **Antibody Sequence Validation by Peptide and Disulfide Bridge Mapping;** Yi Liu¹; Lei Xin²; Baozhen Shan²; Kaizhong Zhang¹; ¹*University of Western Ontario, London, ON*; ²*Bioinformatics Solutions Inc, Waterloo, ON*
- TP 053 **ImmunocaptureLC-HRMS for the Quantitation of Therapeutic Monoclonal Antibody Ipilimumab Using Light Chain Approach;** Yongxin Zhu¹; John Mehl¹; France Landry¹; Srikanth Kotapati²; David Passmore²; Haiqing Wang³; Eugene Ciccimaro Jr. ¹; Timothy Olah¹; ¹*Bristol-Myers Squibb, Princeton, NJ*; ²*Bristol-Myers Squibb, Redwood City, CA*
- TP 054 **Quantitative HPLC-MS/MS Analysis of DM1 and DM1-MCC Extracted from Whole Blood Dried onto a Mitra Microsampling Device;** Chad D. Christianson¹; Michael D. Williams¹; Natalie C. Garcia²; Katherine M. Yahvah¹; ¹*Alturas Analytics, Moscow, ID*; ²*Neoteryx, LLC, Torrance, CA*
- TP 055 **High-Resolution Accurate-Mass LC-MS enables In-**
- Depth Characterization of *in vivo* Biotransformations for Intact Antibody-Drug Conjugates;** Jintang He¹; Dian Su¹; Carl Ng¹; Luna Liu¹; Shang-Fan Yu¹; Thomas Pillow¹; Geoffrey Del Rosario¹; Surinder Kaur¹; Keyang Xu¹; ¹*Genentech, Inc, South San Francisco, CA*
- TP 056 **Application of Non-Reduced Peptide Mapping by Mass Spectrometry (MS) for the Characterization of Site-Specific Cysteine Antibody-Drug Conjugates;** Andrew W. Dawdy¹; Jason C. Rouse²; Olga V. Friese¹; ¹*Pfizer Inc, St Louis, MO*; ²*Pfizer Inc., Andover, MA*
- TP 057 **Assessing Biosimilarity of Eight Different Batches of Commercial Herceptin with Similarity Index Derived from Comprehensive Biophysical Data;** Mowei Zhou¹; Alejandro Heredia-Langner¹; David Bush²; Erika Zink¹; Xueyun Y Zheng¹; Ernesto Nakayasu¹; Erin S Baker¹; Charles Ansong¹; John Cort¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Genedata, Lexington, MA*
- TP 058 **Evaluation of Factors Affecting Detection of Host Cell Proteins in Biotherapeutic Proteins using an Orbitrap Fusion Lumos Tribrid Mass Spectrometer;** Stephane Houel¹; Michael Blank¹; Romain Huguet¹; Seema Sharma¹; Martin Samonig²; Vlad Zabrouskov¹; Jonathan Josephs¹; ¹*Thermo Fisher Scientific, San Jose, California*; ²*Thermo Fisher Scientific, Bremen, Germany*
- TP 059 **Highly Automated Analysis of Antibody Chain Shuffling in Bispecific Antibodies;** Marshall Bern¹; Yong J. Kil¹; Eric Carlson¹; Brian D. Soriano²; Stone D.-H. Shi²; ¹*Protein Metrics Inc., San Carlos, CA*; ²*Amgen, Thousand Oaks, CA*
- TP 060 **Full Validation of Therapeutic Antibody Sequences by Middle-Up Mass Measurements and Middle-Down Protein Sequencing as a Routine Task;** Anja Resemann¹; Wolfgang Jabs²; Elsa Wagner³; Olivier Colas³; Waltraud Evers¹; Jason S. Wood⁴; Eckhard Belau¹; Lars Vorwerk¹; Alain Beck³; Detlev Suckau¹; ¹*Bruker Daltonics, Bremen, Germany*; ²*Beuth University of Applied Sciences Berlin, Berlin, Germany*; ³*Laboratoires Pierre Fabre, Paris, France*; ⁴*Bruker Daltonics, Billerica, MA*
- TP 061 **Pilot Study Regarding Automated Comparative Fd- and Fc-Domain MS-Based Glycoprofiling for High-Throughput Online Process Monitoring of Therapeutic Antibody Production;** Sven Bahrke¹; Robert Wilmanowski¹; Martin Hedström²; Dag Erlandsson²; Fredrik Olsson²; Detlev Suckau³; Wolfgang Jabs⁴; ¹*Glycotope GmbH, Berlin, Germany*; ²*CapSenze Biosystems AB, Lund, Sweden*; ³*Bruker Daltonik GmbH, Bremen, Germany*; ⁴*Beuth University of Applied Sciences Berlin, Berlin, Germany*
- TP 062 **Use Information Independent SWATH Acquisition for Biotherapeutic Peptide Mapping;** Ji Luo; *Shanghai AB Sciex Analytical Instrument Trading Co., Ltd, Shanghai, China*
- TP 063 **BiopharmaView™ Software as a Robust Tool for Automated Quantitation of Oxidation Sites in Monoclonal Antibody Characterization;** Kerstin Pohl¹; Annu Uppal²; Amandine Boudreau³; ¹*SCIEX, Darmstadt, Germany*; ²*SCIEX, Gurgaon, India*; ³*SCIEX, Concord, ON*
- TP 064 **Rapid Method for IgG Met-255 Oxidation Level Determination by LC-MS. Method Development and Qualification;** Tomasz Welerowicz¹; Tomasz Gozdziwicz¹; Radoslaw Obuchowicz¹; Marianna Sztolpa¹; Krystian Siten¹; Pawel Socha¹; Michael Safinowski¹; Piotr Zien¹; ¹*Polpharma Biologics, Gdansk, Poland*
- TP 065 **HRAMS Monitoring of *in-vivo* Protein Biotransformation's: Quantitative Determination of Trastuzumab and Deamidation Products in Human Plasma by MRMHR and SWATH®;** Jason Causon¹; Kees Bronsema²; Nico Van De Merbel²; Peter Bults²; Edwin Hooijschuur²; Martijn Hilhorst²; Milla Neffling¹; Neil Walsh¹; ¹*SCIEX, Warrington, Cheshire*; ²*PRA HealthSciences, Assen, Netherlands*
- TP 066 **Antibody Verification by Protein Immunoprecipitation**



- and Mass Spectrometry (IP-MS) Characterizes Antibody Performance and Identifies Protein-Protein Interactions;** Gregory K. Potts¹; Bhavin Patel¹; Leigh Foster¹; John C. Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL
- TP 067 **Controlled, In-membrane Protein Digestion for Antibody Characterization and Assessment of Structural Changes;** Merlin Bruening¹; Yongle Pang²; Weijing Liu¹; Wenjing Ning²; Nitin Patel³; Gia Jokhadze³; ¹University of Notre Dame, Notre Dame, IN; ²Michigan State University, East Lansing, MI; ³Takara Bio, Mountain View, CA
- TP 068 **Evaluation of a Microfluidic Electrophoresis Device Coupled to an Orbitrap Mass Spectrometer for the Characterization of Biotherapeutics Proteins;** Stephane Houel¹; Erin Redman²; Scott Mellors²; Aaron Bailey¹; Chris Petty³; Aran Paulus¹; Kai Zhou⁴; Jonathan Josephs¹; ¹Thermo Fisher Scientific, San Jose, California; ²908 Devices, Inc., Carrboro, NC; ³908 Devices Inc., Boston, MA; ⁴Thermo Fisher Scientific, Cambridge, MA
- TP 069 **Evaluation of the Arginine Specific Protease RgpB for LC-MS Based Antibody Analysis;** Sheila Maibom-Thomsen^{1,2}; Peter Højrup²; Jakob Bunkenborg¹; Malin Mejare³; Ejvind Mørtz¹; Fredrik Olsson³; Thomas Kofoed¹; Maria Nordgren³; ¹Alphalyse, Odense, Fyn; ²University of Southern Denmark, Odense, Denmark; ³Genovis, Lund, Sweden
- TP 070 **Physicochemical Characterization of an Original and Biosimilar Omalizumab by Mass Spectrometry Methods;** Maksim Degterev¹; Rakhim Shukurov¹; Alexander Vishnevskiy¹; Igor Fabrichniy¹; ¹IBC Generium, Vol'ginsky
- TP 071 **Mass Spectrometry as an Orthogonal Technique to Quality Control and Sequencing in Recombinant mAb Production;** Scott A Robotham¹; Jason Hogan²; Nicole Bracy-Johnson¹; Holly Palme¹; Aarti Jashnani²; Jia Dong²; Billy Akinsanya¹; Adela Buzescu¹; Andy Deng²; Meaghan Happer²; Jonathan R Haulenbeek¹; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Redwood City, CA
- TP 072 **Establishing Translation of a Whole-Molecule LC-MS Assay for in vivo Quantitation of mAbs: From Pharmacokinetic Analyses to Critical Quality Attributes;** John F. Kellie¹; Robert A. Biddlecombe²; Sarah Childs²; Molly Z. Karlinsey¹; ¹GSK, King of Prussia, PA; ²GSK, Stevenage, UK
- TP 073 **Mapping the Effects of UV Irradiation on Monoclonal Antibody Drugs;** J. Larry Campbell¹; Chris Lock¹; Brendon Seale^{2,3}; J.C. Yves Leblanc²; Suyu Liu²; Xu Guo²; Wen Jin²; Michael Sasges⁴; Michelle Gabriel⁴; Mark Schofield⁵; Marc Aucoin⁶; Emma Dare⁶; ¹SCIEX, Concord, ON; ²SCIEX, Concord, ON, ON; ³University of Toronto, Toronto, ON; ⁴Trojan Technologies, London, Ontario; ⁵Pall Corporation, Westborough, MA; ⁶University of Waterloo, Waterloo, Ontario
- TP 074 **Characterization of N-glycans in Therapeutic Glycoproteins by Hydrophilic Interaction Ultra High Performance Liquid Chromatography-Fluorescence-Mass Spectrometry (HILIC-UHPLC-FLD-MS);** Annette Vogt¹; Cornelia Wagner¹; Babette Werner¹; Andreas Adlberger¹; Laurent Lariviere¹; Hans Koll¹; ¹Roche Pharma Research and Early Development (pRED), Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany
- TP 075 **Comparative Fc N-glycosylation Profiling at Glycopeptide Level for Differentiation and Verification of Monoclonal Antibody Therapeutics using HILIC-SPE Coupled to MALDI-TOF-MS;** Lianji Jin; FDA, Cincinnati, OH
- TP 076 **Degradation Study of the NISTmab Reference Material: From the Discovery to Routine Quantification of Stress Related Artefacts;** Guillaume Tremintin¹; Detlev Suckau²; Peter Hufnagel²; ¹Bruker Daltonics, Fremont, CA; ²Bruker Daltonik GmbH, Bremen, Germany
- TP 077 **Multilevel Characterisation of Site-Specific Antibody Drug Conjugates (ADC) using RP-UPLC-ESI-MS ;** Sylwia Jozwiak¹; James Graham¹; ¹Lonza Biologics, Slough, Berkshire
- TP 078 **Determination of Released Payload Species of Antibody Drug Conjugates with Noncleavable Linkers by High Resolution Mass Spectrometry and Metabolite Pilot Software;** Ian Moore¹; Yuan-Qing Xia²; ¹SCIEX, Concord, ON; ²Sciex, Frammingham, MA
- TP 079 **Routine Host Cell Protein (HCPs) Monitoring and Non-Targeted New Feature Detection and Identification as Part of Mass Spectrometry-based Quality Control ;** Michael Blank¹; Stephane Houel¹; Jonathan Josephs¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 080 **Toward de novo Sequencing of Mixtures of Antibodies;** Natalie Castellana¹; Kexin Huang²; Alice Liang²; Siyang Wang²; Hua Tu²; ¹Digital Proteomics, LLC., La Jolla, CA; ²LakePharma, Inc., Belmont, CA
- TP 081 **Automatic End-to-End de novo Sequencing (Including I/L) of Antibodies with ETHcD Fragmentation;** Wilfred H. Tang¹; Yong J. Kil¹; K. Ilker Sen¹; Marshall Bern¹; Shruti Nayak²; Beatrix Ueberheide²; Gregg Silverman²; ¹Protein Metrics, San Carlos, CA; ²New York University Langone Medical Center, New York, NY
- TP 082 **Automated Determination of ADC Drug-Antibody Ratios Using an Open Access System;** Tanner Stevenson¹; Stephen Madden²; David Wong²; Jade C. Byrd²; Robert Williams²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies Inc., Santa Clara, CA
- TP 083 **Practical Glycan Analysis: Comparison of Methods for Characterizing Glycan Profiles of Recombinant Monoclonal Antibodies;** Loredana Serafini¹; Gregory Staples²; Caroline S. Chu²; Andy Gieschen²; Adele Taylor³; Greg Tuffy¹; Mark Nagel¹; Cody Williams⁴; Justin Golde⁴; Gregg Czerwieniec¹; Katherine M. Brenda⁴; Roman Sakowicz¹; ¹Gilead Sciences, Foster City, CA; ²Agilent Technologies, Inc., Santa Clara, CA; ³ProZyme, Hayward, CA; ⁴Hamilton Robotics, Reno, Nevada
- TP 084 **Fast Stability Assessment of a Next Generation Antibody Drug Conjugate by N-Acetylcysteine-Drug Conjugate Model Compound Degradation Study;** Chunang (Christine) Gu¹; Omar Hamdy¹; John Peattle¹; Ieiza Danan-leon¹; Tony Cano¹; ¹Abbvie Stemcentrx LLC, South San Francisco, CA
- TP 085 **A Novel LC/MS-based Pipeline Enabling Comprehensive Investigation of Tumor/Tissue Disposition of Antibody-Drug-Conjugate, in vivo DAR, Free Toxin and Antigen Turnover;** Bo An¹; Ming Zhang¹; Yang Qu¹; Yuan-ju Chen¹; Jun Qu¹; ¹SUNY at Buffalo, Buffalo, NY
- TP 086 **Profiling the N-Glycosylation of Biotherapeutic IgGs with HILIC-MRM Analysis of Trypsin Digested Culture Media;** Ron Orlando^{1,2}; Gerardo Gutierrez²; Tyler Fletcher³; ¹University of Georgia, Athens, GA; ²GlycoScientific, LLC, Athens, GA; ³University of Georgia, Athens, GA
- TP 087 **Improved Top-Down and Middle-Down Characterization of Antibodies using Multiple Ion Activation Techniques on a Modified Orbitrap Tribrid Mass Spectrometer;** Luca Fornelli¹; Kristina Szentić¹; Romain Huguet²; Stephane Houel²; Aaron Bailey²; Helene Cardasis²; Ryan T. Fellers¹; Tara Schroader²; Horn M. David²; Seema Sharma²; Philip D. Compton¹; Jonathan Josephs²; Vlad Zabrouskov²; Mike Senko²; Neil L. Kelleher¹; ¹Northwestern University-Kelleher Research Group, Evanston, IL; ²Thermo Fisher Scientific, San Jose, CA
- TP 088 **N-linked Glycan Profiling for Monoclonal Antibodies using Bottom-Up and Middle-Down LC-MS Approaches;** Lin He¹; Jonathan Krieger²; Paul Taylor²; Baozhen Shan¹; ¹Bioinformatics Solutions Inc, Waterloo, ON; ²Hospital for Sick Children, Toronto, Ontario
- TP 089 **LC-MS/MS Quantitative Method Development of**



Herceptin Based on nSMOL Technology and Skyline Software; Hongyuan Hao¹; Qiaoxia Liu¹; Taohong Huang¹; ¹Shimadzu (China) Co.,Ltd., Shanghai

BIOMARKERS: QUANTITATIVE ANALYSIS I
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- TP 090 **A HILIC-MS/MS Method for Simultaneous Quantification of the Lysosomal Disease Markers Galactosylsphingosine and Glucosylsphingosine in Mouse Serum;** Xuntian Jiang; Diabetic Cardiovascular Disease Center, Washington, St. Louis, MO
- TP 091 **Bioanalytical Method Development for the Determination of Desmosine and Isodesmosine in Mouse Urine by ion-pair reverse phase LC-MS/MS;** Philip S. Wong¹; Jian Jiang¹; Christopher A James¹; ¹Amgen, Thousand Oaks, CA
- TP 092 **Absolute Quantification of Site-Specific Core-Fucosylation of Serum Fibronectin in Alcohol-Related Hepatocellular Carcinoma;** Haidi Yin¹; David M. Lubman²; Zhongping Yao¹; ¹The Hong Kong Polytechnic University, Hong Kong, China; ²University of Michigan, Ann Arbor, MI
- TP 093 **A fast and Sensitive LC-MS/MS Method for the Determination of Lyso-Gb3 in Human Plasma;** Wuyi (Charlie) Zha¹; Karolina Doda¹; Mohamed Osman¹; Xinping Fang¹; ¹WuXi AppTec, Inc, Plainsboro Township, NJ
- TP 094 **Quantitative Proteomic Analysis of Serum Exosomes from Patients with locally Advanced Pancreatic Cancer Undergoing Chemoradiotherapy;** Mingrui An¹; Kyle C. Cuneo¹; Jianhui Zhu¹; Jing Wu¹; Jing Liang¹; Mengmeng Wang¹; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- TP 095 **Quantification Performance of Non-Invasive LC-MS/MS Analysis and Evaluation of Undifferentiated State of Human iPS Cells;** Kenichi Toyoda¹; Takashi Suzuki¹; Kunitada Hatabayashi²; Kenichi Kagawa²; Masatoshi Takahashi¹; ¹Shimadzu Corporation, Nakagyo-ku, Japan; ²Tokyo Electron Limited, Minato-ku, Japan
- TP 096 **Biomarker Monitoring by Quantitative MALDI Imaging: Application to the Tryptophan-Kynurenine Pathway in Immuno-Oncology;** Rima Ait-Belkacem¹; Vanesa Bol²; David Bonnel¹; Bruno Gomes²; Jonathan Stauber¹; ¹Imabiotech, Loos, France; ²Teos Therapeutics SA, Gosselies, Belgium
- TP 097 **Investigation of Protective Mechanism of a Bacterial Mixture of Human Commensals against Colon Tumorigenesis by Quantitative Proteomics Analysis;** Jing Wu¹; Mingrui An¹; Jianhui Zhu¹; Grace Y. Chen¹; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- TP 098 **Verification of Genomics Biomarker Candidates for Prostate Cancer at the Protein Level Using SRM-MS;** Hui Wang¹; Yuqian Gao¹; Athena schepmoes¹; Gyorgy Petrovics²; Jennifer Cullen²; Thomas Fillmore¹; Tujin Shi¹; Wei-Jun Qian¹; Richard Smith¹; Brandi Weaver³; Robin Leach³; Ian Thompson³; Sudhir Srivastava⁴; Albert Dobi²; Karin Rodland¹; Jacob Kagan⁴; Shiv Srivastava²; Tao Liu¹; ¹PNNL, Richland, wa; ²Uniformed Services University of the Health Sciences, Bethesda, MD; ³Univerysity of Texas Health and Science Center at San Antonio, San Antonio, TX; ⁴National Cancer Institute, Bethesda, MD
- TP 099 **Quantitative Targeted-SIM Assay for Neuron-specific Enolase in Small-cell Lung Cancer using Formalin-fixed Paraffin-embedded Tissue Samples;** Kiyonaga Fujii¹; Yuka Miyata²; Ikuya Takahashi²; Hirotaka Koizumi¹; Hiromasa Tojo¹; Hisashi Saji¹; Toshiaki Somehara^{1,2}; Masayuki Takagi¹; Haruhiko Nakamura¹; Toshihide Nishimura¹; ¹St. Marianna University School of Medicine, Kawasaki, Japan; ²Nissha Printing Co., Ltd., Kyoto, Japan
- TP 100 **N-glycopeptides Analysis of Serum Alpha-1-antitrypsin**

- in Liver Cirrhosis and Hepatocellular Carcinoma;** Mengmeng Wang^{1,2}; Jianhui Zhu¹; Jing Liang^{1,3}; Tingting Chen¹; Mingrui An¹; Yifan Huang⁴; Yehia Mechref⁴; Chunfang Gao²; David M. Lubman¹; ¹Department of Surgery, University of Michigan Medical Center, Ann Arbor, MI; ²Department of Laboratory Medicine, Eastern Hepatobiliary Surgery Hospital, Second Military Medical University, Shanghai, China; ³School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou, China; ⁴Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX
- TP 101 **Improved Sensitivity for Protein Biomarker Quantitation in Mouse Plasma by Sample Pretreatment and Trap-Elute Micro-Flow LC-MS/MS;** Mingfei Zeng¹; Huachuan Cao¹; ¹Eli Lilly and Company, Shanghai, China
- TP 102 **The Power of Quantitative Multiplexing- Combining TMT Discovery and Targeted Label Free Workflows for Biomarker Analysis;** Xiaoyue Jiang¹; Katherine Herting²; Ramesh Ganapathy²; Sergei Snovidat²; David Horn³; Vic Spicer⁴; Oleg Krokhn⁴; Rosa Viner⁵; Andreas F. Huhmer⁵; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Rockford, IL; ³Thermo Fisher Scientific, San Jose, CA; ⁴University of Manitoba, Winnipeg, MB; ⁵Thermo Fisher Scientific, San Jose, CA
- TP 103 **Quantitation of Stercobilin in the Fecal Material of Timothy Syndrome Mice as a Putative Biomarker for Autism;** Emily Sekera¹; Troy D. Wood¹; Heather L Rudolph¹; Stephen Carro¹; ¹University at Buffalo, Buffalo, NY
- TP 104 **Oxyntomodulin Quantitation in Human Plasma: High Resolution Q-TOF Quantification Myths Debunked;** Megan Yajuan Wang¹; Anita Lee¹; Derek Chappell¹; Omar Laterza¹; Michael Lassman¹; ¹Merck Research Laboratories, Rahway, NJ
- TP 105 **Monitoring with Quantitation the Glycosylation of Multiple Glycoproteins for Diseases Biomarker Discovery;** Qiongyu Li¹; Muchena J. Kailemia¹; Frank Leon²; Emanuel Maverakis³; Carlito B. Lebrilla¹; ¹Department of Chemistry, University of California, Davis, Davis, CA; ²Biochemistry, Molecular, Cellular and Developmental Biology, University of California, Davis, Davis, CA; ³Department of Dermatology, School of Medicine University of California, Davis, Sacramento, CA
- TP 106 **Site-Specific Glycopeptide Analysis of Human alpha-1-acid Glycoprotein (AGP) in Liver Cirrhosis and Hepatocellular Carcinoma of Different Etiologies;** Jing Liang^{1,2}; Jianhui Zhu³; Mingrui An³; Mengmeng Wang³; ⁴Yifan Huang⁵; Yehia Mechref⁶; David M. Lubman⁷; ¹University of Michigan Medical Center, Ann Arbor, Michigan; ²School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou, China; ³University of Michigan Medical Center, Ann Arbor, MI; ⁴Department of Laboratory Medicine, Eastern Hepatobiliary Surgery Hospital, Second Military Medical University, Shanghai, China; ⁵Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX; ⁶Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX; ⁷University of Michigan Medical Center, Ann Arbor, MI
- TP 107 **Oxysterol, Secosterols, and Cholesterol Intermediates Separation and Quantitation Using Triple Quadrupole Mass Spectrometry;** Evelyn H. Wang¹; Jerry Byrne II¹; Rachel Lieberman¹; Sonia Bholanath Bhattacharya²; Richard W. Browne²; Christopher Gilles¹; ¹Shimadzu Scientific Instruments, Columbia, MD; ²University of Buffalo, Buffalo, NY
- TP 108 **Orthogonal Proteomic Verification of Low Histone H4-K12,16Ac Levels in Homologous Recombination Deficient High-Grade Serous Ovarian Carcinomas;** Stefani Thomas¹; Lijun Chen¹; Yang Liu¹; Naseruddin Höti¹; Hui Zhang¹; ¹Johns Hopkins University, Baltimore, MD
- TP 109 **Capillary Electrophoresis-Mass Spectrometry**



Method Development for Biomarkers of Indoleamine 2,3-Dioxygenase; Yunan Wang¹; Mei Han¹; Jing Man Wong¹; Dan A. Rock¹; Brooke M. Rock¹; ¹Amgen, South San Francisco, CA

- TP 110 **Alpha-1 Antitrypsin Quantification using LC-MS/MS;** Qingguo Tian¹; Bob Xiong²; Eric Lund¹; Dawn Christianson¹; Zhen Li¹; ¹Arrowhead Pharmaceuticals Inc., Madison, WI; ²Covance, Durham, NC
- TP 111 **Mass Spectrometry based Proteomics Investigation of Induced Obstructive Sleep Apnea (OSA) in Rat Atria;** Devika Channaveerappa¹; Jacob Lux²; Kelly L. Wormwood²; Meredith McLerie²; Brian Panama²; ¹Clarkson University, Potsdam, NY; ²Masonic Medical Research Laboratory, Utica, NY

CARBOHYDRATES II 112 - 137

- TP 112 **Mass Spectrometry Profiling of Pentosan Polysulfate;** Komal Kedia¹; Xueyun Xheng¹; Mowei Zhou¹; Charles Ansong¹; Erin S Baker¹; John Cort¹; ¹PNNL, Richland, WA
- TP 113 **Fast Pyrolysis of 13C- and 18O-Labelled Cellobiosaccharides: Probing the Mechanisms of Fast Pyrolysis of Carbohydrates by Using Tandem Mass Spectrometry;** Zaikuan Yu¹; Priya Murria¹; Mckay Easton¹; Hilikka Kenttämää¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN
- TP 114 **Structural Characterization of Heparin and Heparan Sulfate using 193 nm Ultraviolet Photodissociation;** Dustin Klein¹; Jennifer S Brodbelt²; ¹University of Texas at Austin, Austin, TX; ²University of Texas at Austin, Austin, TX
- TP 115 **Resolution of Carbohydrate Isomers via Ion Mobility-Mass Spectrometry with Boronic Acid Shift Reagent;** Li Li¹; Kristin M McKenna¹; Facundo M Fernandez¹; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA
- TP 116 **Evaluation of UV Detection as a Novel Method for Glycan Analysis;** Charles Nwosu¹; Shuangqi Sally Liu¹; May Zhu¹; ¹Takeda Pharmaceuticals International, Cambridge, MA
- TP 117 **Linkage and Anomeric Configuration Determination by Electrospray Ionization Tandem Mass Spectrometry;** Chia Yen Liew¹; Shang-Ting Tsai¹; Jien-Lian Chen¹; Hsu Chen Hsu¹; Shih-Pei Huang¹; Yuan-Tseh Lee^{1,2}; Chi-Kung Ni^{1,3}; ¹Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; ²Department of Chemistry, National Taiwan University, Taipei, Taiwan; ³Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan
- TP 118 **Machine Learning Approach for de novo Glycan Sequencing;** Pengyu Hong¹; Yang Tang²; Hui Sun¹; Long Sha¹; Catherine E Costello^{2,3}; Cheng Lin³; ¹Brandeis University, Waltham, MA; ²Boston University, Boston, MA; ³Boston University School of Medicine, Boston, MA
- TP 119 **High Mannose Glycan Characterization and Quantitation by Free Radical Reagents;** Kimberly Fabijanczuk¹; Jose Acosta²; Trang Do²; Jinshan Gao²; ¹Montclair, NJ - New Jersey; ²Montclair State University, Montclair, NJ
- TP 120 **Glycan Characterization and Quantitation by Free Radical Reagents;** Jinshan Gao¹; Kaylee Gaspar¹; Trang Do¹; Nathaniel Adomako¹; Kimberly Fabijanczuk¹; Jose Acosta¹; ¹Montclair State University, Montclair, NJ
- TP 121 **A Rapid LC-MS/MS-based Method for Carbohydrate Linkage Identification Using Multiple Reaction Monitoring (MRM);** Ace G. Galermo¹; Eshani Nandita¹; Mariana Barboza^{1,2}; Matthew J. Amicucci^{1,3}; Thai-Thanh Vo¹; Carlito B. Lebrilla¹; ¹Department of Chemistry, University of California, Davis, Davis, CA; ²Department of Anatomy, Physiology, and Cell Biology, University of California, Davis, Davis, CA; ³Agricultural and Environmental Chemistry Graduate Group, University of California, Davis, Davis, CA
- TP 122 **Novel 4-plex Isobaric Aldehyde Reactive N, N-Dimethyl**

- Leucine Derivative Tags for Quantitative Glycomics Analysis;** Yu Feng¹; Bingming Chen¹; Qinying Yu¹; Xuefei Zhong¹; Lingjun Li^{1,2}; ¹University of Wisconsin-Madison School of Pharmacy, Madison, WI; ²University of Wisconsin - Madison Department of Chemistry, Madison, WI
- TP 123 **Comparative Study of in-ESI, Solution-Phase, and Gas-Phase Hydrogen/Deuterium Exchange for Conformational Analysis of Carbohydrate-Metal Adducts;** Tara Liyanage¹; Matthew R Brantley¹; Touradj Solouki¹; Elyssia S Gallagher¹; ¹Baylor University, Waco, TX
- TP 124 **Sialyl Glycan Characterization by Free Radical Activated Glycan Structure Elucidation Reagent;** Kaylee Gaspar¹; Trang Do²; Nathaniel Adomako²; Jinshan Gao²; ¹Montclair, NJ; ²Montclair State University, Montclair, NJ
- TP 125 **Absolute Quantitation of Branching in Polysaccharides using Isotopically Differentiated Permethylolation;** Eshani Nandita¹; Ace G. Galermo¹; Matthew J. Amicucci²; Mariana Barboza³; Carlito B. Lebrilla¹; ¹UC Davis Department of Chemistry, Davis, CA; ²UC Davis Agricultural and Environmental Chemistry Graduate Group, Davis, CA; ³UC Davis Department of Anatomy, Physiology, and Cell Biology, Davis, CA
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- TP 127 **New Applications and Technologies for INLIGHT™ N- and O-linked Glycans;** Samuel R. King¹; Elizabeth S. Hecht¹; Philip L. Loziuk¹; Erin S. Baker²; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²Pacific Northwest National Laboratory, Richland, WA
- TP 128 **Formation of Doubly Alkali Metal-Cationized Monosialylated Fragments from Singly Alkali Metal-Cationized LSTb and GM1 during MALDI-MS/MS and ESI-MS/MS;** Krishani K. Rajanayake¹; Kevin Markus¹; Dragan Isailovic¹; ¹The University of Toledo, Toledo, OH
- TP 129 **Structural Elucidation of Fucosylated Chondroitin Sulfates from Sea Cucumber Using Electrospray Ionization Tandem Mass Spectrometry;** Isaac Agyeekum¹; Lauren Pepi¹; Shiguo Chen²; Robert J Linhardt³; I Jonathan Amster¹; ¹University of Georgia, Chemistry Department, Athens, GA; ²Zhejiang University, Department of Food Science and Nutrition, Hangzhou, China; ³Rensselaer Polytechnic Institute, Troy, NY
- TP 130 **Sensitive Detection of Sialylated N-Glycans using Optimized HILIC LC-MS Separations;** Qi Wang¹; Matthew A. Lauber¹; ¹Waters Corporation, Milford, MA
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- TP 132 **Optimization of Reverse Polarity Capillary Electrophoresis-Mass Spectrometry Separations for the Analysis of Sulfated Glycosaminoglycan Oligosaccharide Mixtures;** Morgan Stickney¹; Patience Sanderson¹; Franklin E Leach III¹; James Xia²; Yanlei Yu³; Fuming Zhang³; Robert J Linhardt³; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²CMP Scientific, Corp., Brooklyn, N.Y.; ³Rensselaer Polytechnic Institute, Troy, NY
- TP 133 **Negative Electron Transfer Dissociation Sequencing of Increasingly Sulfated Glycosaminoglycan Oligosaccharides in an Orbitrap Mass Spectrometer;** Franklin E. Leach III¹; Nicholas M. Riley²; Matthew J. P. Rush²; Michael S. Westphall²; Joshua J. Coon²; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²University of Wisconsin, Madison, WI
- TP 134 **Rapid and Sensitive MALDI MS Analysis of**



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- TP 136 **From Computation to Mass Spectrometry: Relative Free Energy Differences amongst Anomeric Pairs of Carbohydrate Derivatives;** Gabe Nagy¹; Alison E. Vickman¹; Nicola L. B. Pohl¹; ¹Indiana University Bloomington, Bloomington, IN
- TP 137 **Does Low Energy CID Always Occur on the Reducing End of Carbohydrate?** Shang-Ting Tsai¹; Chia Yen Liew²; Shih-Pei Huang²; Yuan-Tseh Lee^{2,3}; Chi-Kung Ni^{2,4}; ¹Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; ²Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; ³Department of Chemistry, National Taiwan University, Taipei, Taiwan; ⁴Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan
- TP 138 **Incorporating Mass Spectrometry into Biologic QC Control Environments for O- Glycan Analysis;** Mark Hilliard¹; Ciara McManus¹; William Alley²; Ying Qing Yu²; Pauline Rudd¹; ¹NIBRT, Dublin, Ireland; ²Waters Corporation, Milford, MA

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- TP 139 **Analysis of Protein-Protein Interactions by Data-Dependent Acquisition without Dynamic Exclusion;** Shen Zhang¹; Brett Larsen²; Anne-Claude Gingras²; ¹Lunenfeld-Tanenbaum Research Institute, Toronto, Ontario; ²Lunenfeld-Tanenbaum Research Institute, Toronto, ON
- TP 140 **Developing and Executing Advanced Data-Dependent Acquisition Strategies for Proteomics in MaxQuant-RealTime;** Christoph Wichmann¹; Florian Meier¹; Matthias Mann¹; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 141 **Evaluation of a Peptide Selection Algorithm for Trapped Ion Mobility with Parallel Accumulation Serial Fragmentation (TIMS-PASEF) on a Q-TOF Instrument;** Markus Lubeck¹; Stephanie Kaspar-Schoenefeld¹; Niels Godecke¹; Oliver Raether¹; Scarlet Beck²; Heiner Koch²; Florian Meier²; Juergen Cox²; Matthias Mann²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 142 **Laser-Induced Dissociation Combined with Data Independent Acquisition (DIA-LID) : A Proof of Concept Study Covering Human Kinome Expression;** Lény Garcia¹; Marion Girod¹; Magali Rompais²; Philippe Dugourd³; Christine Carapito²; Jérôme Lemoine¹; ¹Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France; ²Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; ³Institut Lumière Matière, Université de Lyon, Université Lyon 1, CNRS, Lyon, France
- TP 143 **Deciphering Heterochromatin Proteome with Next Generation Proteomics;** Tania Auchynnikava¹; Lauri Peil²; Piotr Grabowski³; Alison Pidoux⁴; Ryan Ard⁴; Robin Allshire⁴; Juri Rappsilber^{3,4}; ¹University of Edinburgh, Edinburgh; ²University of Tartu, Tartu, Estonia; ³Technical University Berlin, Berlin, Germany; ⁴University of Edinburgh, Edinburgh, UK
- TP 144 **Maximizing Proteome Coverage through Judicious Selection of Quadrupole Ion Trap Settings and Improved On-Line Orbitrap Peak Annotation;** Graeme McAlister¹; Christian Thoeing²; Romain Huguet¹; Alex Hebert³; Philip M Remes¹; Andreas Kuehn²; Vlad Zabrouskov¹; Joshua J. Coon³; Mike Senko¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bremen, Germany; ³University of Wisconsin Madison, Madison, WI
- TP 145 **The Advantages of Using an MRMHR Acquisition for Increased Sensitivity for Targeted Analysis Using a QTOF Instrument;** Paul C. Winkler¹; K.C. Hyland²; Christopher Borton²; ¹SCIEX, Framingham, MA; ²SCIEX, Redwood City, CA

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- TP 150 **Evaluation of Noviplex Card for Plasma Concentration Determination;** Lingling Xue¹; Yang Xu¹; James Schiller¹; guangping Bi¹; Michelle Groff¹; Jane Harrelson¹; ¹Merck & Co., Inc., West Point, PA
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- TP 152 **Experimental Investigation of the Factors Affecting the Sensitivity of HPLC/MS Coupled with Ion-Molecule Reactions;** Ravikiran Yerabolu¹; Raghavendhar R Kotha¹; John Kong¹; Zaikuan Yu¹; Rashmi Kumar¹; Chungang Gu²; Hilkka Kentamaa¹; ¹Purdue University, West Lafayette, IN; ²AstraZeneca R&D, Waltham, MA
- TP 153 **Development of High-Performance Micro-flow LC-MS/MS Methodology and Application to a High-Throughput Screening Workflow;** Brendon Kapinos¹; John Janiszewski¹; Hui Zhang¹; Jianhua Liu¹; Brian Holder¹; Wayne Lootsma²; Steve Ainley²; Amanda Berg³; Erik Hansen³; ¹Pfizer Inc., Groton, CT; ²Sound Analytics, Niantic, CT; ³New Objective, Woburn, MA
- TP 154 **Understanding Metabolism of an Achiral Drug to Chiral Metabolites in Biological Matrices using SFC-QQQ Technology;** Siji Joseph¹; Syed Salman Lateef²; ¹Agilent technologies, Bangalore, Karnataka; ²Agilent Technologies India, Bangalore, India
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- TP 156 **Comparison of Combining Quantitative with Qualitative Met ID Analysis in the QTrap 6500 and Triple TOF 5600 Mass Spectrometer**; Minli Zhang¹; Keith J. Goodman²; Diane L. Nabb¹; Heather Peterson¹; John M. Hevko²; ¹DuPont, Newark, DE; ²Sciex, Frammingham, MA
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- TP 158 **High-Resolution Mass Spectrometry for Efficient Identification of the Transformation Products of Aromatic Emerging Contaminants in Chlorinated Water**; Wen-Ling Chen¹; Jiun-Yi Cheng¹; ¹Department of Environmental Science and Engineering, College of Engineering, Tunghai University, Taichung, Taiwan
- TP 159 **Application of Paper Spray Differential Ion Mobility Mass Spectrometry for Pesticide Products Screening**; Khang To; University of North Carolina, Chapel Hill, NC
- TP 160 **MS-MS Studies of the Partitioning and Recovery of Pesticides Interacting with Soils**; Heather Gamble¹; Miles Snow²; Donald S Gamble³; ¹Perkin Elmer Health Sciences, Bolton, ON; ²PerkinElmer LAS Canada Inc, Woodbridge, ON; ³Department of Chemistry, St. Mary's University, Halifax, NS
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- TP 164 **High-Speed Formaldehyde Analysis for the Process-Line and Laboratory: SIFT-MS**; Murray J Mcewan¹; Mark Perkins²; Daniel B Milligan³; Barry J Prince³; Vaughan S Langford³; ¹University of Canterbury, Christchurch, Canterbury; ²Anatune Limited, Cambridge, UK; ³Syft Technologies Ltd, Christchurch, New Zealand
- TP 165 **Improved Quantitation of Fragile Carbamate, Organophosphate, and Other Pesticides by Automatic MS/MS Method Generation**; Eric Huang¹; Bennett Kalafut¹; ¹Thermo Fisher Scientific, San Jose, CA
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- TP 170 **Analysis of Genotoxic Impurities Like Ethane Sulfonic Acid Esters in Pharmaceutical Substance by GCMS/MS**; Prashant Hase¹; Ankush Bhone¹; Durvesh sawant¹; Dheeraj Handique¹; Sanket Chiplunkar¹; Nitish Suryawanshi¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- TP 171 **A New, Fast, Simple, and Ultra-Sensitive Determination of Semi-Volatile Organic Compounds in Water Samples by GC-MS/MS Triple Quadrupole System**; Diego Martín-Ortiz¹; Javier López¹; Miguel Ángel Pérez¹; Cory Lytle²; Louis Maljers²; ¹Bruker Espanola S.A., Madrid, Spain; ²Bruker Daltonics Inc., Billerica, MA
- TP 172 **Determination of Pesticide Residues for Quality Control of Tobacco Products by LC/MS/MS**; Prasanth Joseph¹; Samir Vyas²; ¹Agilent Technologies, Bangalore, India; ²Agilent Technologies India, Manesar, India
- TP 173 **New Platforms for Environmental (Bio)monitoring**; Geuncheol Gil¹; Pan Mao¹; Daojing Wang¹; ¹Newomics Inc., Emeryville, CA
- TP 174 **Ultra-trace Analytical Method for the Quantification of Pyrethroid and Organophosphate Insecticides in Surface Water using Passive Sampler Membranes and GC-APCI-MS/MS**; Birgit Beck¹; Christoph Moschet²; Juliane Hollender¹; Heinz Singer¹; ¹Eawag, Dübendorf, CH; ²Cantonal Laboratory for the Environment, Schaffhausen, Switzerland
- TP 175 **Isolation and Identification of Priority Contaminants of Emerging Concern and Their Transformation Products: Use of UPLC QToF MS/MS**; Hlengilizwe Nyoni¹; Bhekile B. Mamba¹; Titus A.M. Msagati¹; ¹University of South Africa, College of Science Engineering and Technology, Nanotechnology and Water Sustainability, UNISA Science Campus, Florida, Johannesburg, South Africa
- TP 176 **Measuring Emerging Contaminant Degradation in Anaerobic Digestion or Composting Systems by Liquid-Liquid Extraction and LC-QQQ-MS**; Lisa Wolfe¹; Vicki Larson²; Corey D. Broeckling³; Jessica E. Prenni³; Susan DeLong²; ¹Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO; ²Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO; ³Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO
- TP 177 **Liquid Chromatography-High Resolution Mass Spectrometry as a Powerful Tool of High Volume Screening of Emerging Contaminants in Wastewater**; Alice Tendai Hungwe¹; Vimbai Mhuka¹; Simiso Dube-Nindi¹; Mathew Nindi²; ¹Department of Chemistry, College of Science, Engineering and Technology, the Science Campus, University of South Africa, Florida Park, Roodepoort, Johannesburg, 1709, South Africa, South Africa; ²University of South Africa, Pretoria, Gauteng
- TP 178 **Automated Online SPE/Tandem-MS Analysis of Trace Organic Contaminants in Drinking Water**; Patrick M Batoun¹; Theresa Sosienski²; Dan-Hui Dorothy Yang²; Tarun Anumol³; Craig Marvin³; Patrick Jeanville²; ¹Agilent Technologies Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Santa Clara, CA; ³Agilent Technologies, Inc., Wilmington, DE
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- TP 182 **Pharmaceuticals and Personal Care Products (PPCPs) in Surface Water;** Jerry Byrne II¹; Evelyn Wang¹; Christopher Gilles¹; ¹Shimadzu Scientific Instruments, Columbia, MD
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- TP 185 **Multi-residue Analysis of 18 Regulated Mycotoxins by LC-MS/MS in Food Samples;** David Baker¹; Chris Titman¹; Jonathan Horner²; Neil Loftus¹; Bart Jansen³; ¹Shimadzu, Manchester, UK; ²Scientific Analysis Laboratories, Cambridge, UK; ³Shimadzu Benelux, Hertogenbosch, Netherlands
- TP 186 **Analyzing Spent Grains as a Sustainable Source of Feed;** Liesl Krone¹; BJ Bench²; Manju Bala³; Andre Schreiber⁴; Jennifer Krone⁵; Oscar Cabrices⁶; ¹Granbury High School, Granbury, TX; ²Food Safety and Research Laboratory Tyson Foods, Springdale, AR; ³CPS, PLLC, Brentwood, TN; ⁴SCIEX, Darmstadt, Germany; ⁵SCIEX, Redwood City, CA; ⁶GERSTEL, Inc, Linthicum, MD
- TP 187 **Determination of Mancozeb in Flammulina Velutipes by UPLC-MS/MS;** Guihong Cheng¹; Xiang Li²; Feng Qin³; Cai Chengyuan²; Lizhong Yang²; Zhou Xiangdong²; ¹Sichuan FDA, Chengdu, China; ²PerkinElmer Management (Shanghai) Co, Shanghai, China; ³PerkinElmer LAS Canada Inc, Woodbridge
- TP 188 **Simultaneous Determination of Pesticides Residues and Illegal Additives in Wine by Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry;** Minli Zhu¹; Weifeng Zhang¹; Lina Tang²; Lizhong Yang³; Xiangdong Zhou³; Chengyuan Cai³; Feng Qin⁴; Xiang Li³; Yongming Xie³; ¹Guangzhou Agricultural Products Quantity and Safety Supervisory Institute, Guangzhou, China; ²Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; ³PerkinElmer Management (Shanghai) Co, Shanghai, China; ⁴PerkinElmer LAS Canada Inc, Woodbridge, ON
- TP 189 **Determination of Polycyclic Aromatic Hydrocarbons in Seafood and Edible Oil by Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry;** Min Wu¹; Jin Zhang¹; Lizhong Yang²; Chengyuan Cai²; Xiangdong Zhou²; Zhuo Man²; Feng Qin³; Xiang Li²; Yongming Xie²; ¹Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; ²PerkinElmer Management (Shanghai) Co., Ltd. Shanghai, China, Shanghai, China; ³PerkinElmer LAS Canada Inc, Toronto, ON
- TP 190 **Analysis of Pesticide Residues in Cannabis Regulated by Oregon State using LC-MS/MS;** Sharanya Reddy¹; Ben Armstrong²; Steve Stadlmann²; Toby Astill³; ¹PerkinElmer, Shelton, CT; ²Juniper Labs, Bend, Oregon; ³PerkinElmer Inc., San Jose, CA
- TP 191 **Pesticide Analysis in Hops and Cannabis by GC-MS-MS;** Jeff Dahl¹; Riki Kltano²; Julie Kowalski³; ¹Shimadzu, Columbia, MD; ²Shimadzu Scientific Instr., Columbia, MD; ³Restek Corporation, Bellefonte, PA
- TP 192 **Solid Phase Extraction Based Pass-Through Clean-Up for Multi-Class Analysis of Veterinary Drugs in Baby Food Containing Milk Powder using LC-MS/MS;** Ujwal Patil¹; Sarah Ruiz¹; Cheryl Stephenson¹; John Reuther¹; ¹Eurofins CAL, New Orleans, LA
- TP 193 **Identification of Sweeteners in E-liquids by Electrospray Ionization Mass Spectrometry;** Katherine D. Murdoch¹; James E. Keating¹; Nicholas J. Wallbillich¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC
- TP 194 **Applying 'MRM Spectrum Mode' and Library Searching for Enhanced Reporting Confidence in Routine Pesticide Residue Analysis;** David Baker¹; Chris Titman¹; Jonathan Horner²; Neil Loftus¹; ¹Shimadzu, Manchester, UK; ²Scientific Analysis Laboratories, Cambridge, UK
- TP 195 **Analysis of Toxic Elements in Processed Milk Products using Inductive Coupled Plasma Mass Spectrometry (ICPMS);** Mangesh Pawar¹; Sampada Khopkar¹; Ankush Bhone¹; Amol Shinde¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; ¹Shimadzu Analytical India Pvt. Ltd., Mumbai, Maharashtra
- TP 196 **The Analysis of Polar Ionic Pesticides by Ion-Exchange Chromatography Tandem Mass Spectrometry: The Possible Solution to a Longstanding Problematic Analysis?** Jonathan Beck¹; Stuart Adams²; Michael Dickinson²; Ed George³; Jonathan Guest²; Richard Fussell⁴; ¹ThermoFisher Scientific, San Jose, CA; ²FERA, Sand Hutton, UK; ³ThermoFisher, San Jose, CA; ⁴Thermo Fisher Scientific, Bremen, Germany
- TP 197 **Analysis of Mycotoxins in Food Matrices using HPLC/MS/MS;** Theresa Sosienski¹; Dan-Hui Dorothy Yang¹; Joan Stevens²; Christian Hegmanns³; Patrick Jeanville¹; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Wilmington, DE; ³Agilent Technologies Sales & Services GmbH & Co. KG, Waldbronn, Germany
- TP 198 **Multi-residual Quantitative Analytical Method for Antibiotics in Sea Food by LC/MS/MS;** Anant Lohar¹; Shailendra Rane¹; Rashi Kochhar¹; Ashutosh Shelar¹; Shailesh Damale¹; Purushottam Sutar¹; Deepti Bhandarkar¹; Ajit Datar¹; Pratap Rasam¹; Jitendra Kelkar¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- TP 199 **Target Screening of Multi-Class Antibiotic Residues in Raw Milk using UHPLC Electrospray Ionization Orbitrap Mass Spectrometry;** Daniel Leung¹; Jian Wang¹; Willis Chow¹; James Chang²; ¹Canadian Food Inspection Agency, Calgary, Alberta; ²Thermo Fisher Scientific, San Jose, CA
- TP 200 **I Knew You Were Trouble: Expanding LC Methods to Include Difficult GC Compounds using a Novel Ionization Technique;** Susan Leonard¹; Kari Organtini¹; Gareth Cleland¹; Gordon Fujimoto²; Kenneth Rosnack¹; Ramesh P Rao³; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA; ³Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- TP 201 **Sensitive and Specific Allergen Screening Analysis Using LC-MS/MS;** Paul C. Winkler¹; Hua-Fen Liu²; Christopher Borton²; Leesun New²; ¹Sciex, Framingham, MA; ²SCIEX, Redwood City, CA
- TP 202 **Simultaneous Analysis of Major Allergens in Food Matrices by High Sensitive Mass Spectrometer;** Tairo Ogura; Shimadzu Scientific Instruments, Inc., Columbia, MD
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- TP 204 **Development of a Multi-Residue Confirmatory Method for Determination of Sedatives by HPLC-MS/MS;** Pavel Metalnikov¹; Ilya Batov¹; Renat Selimov¹; Alexander Komarov¹; ¹VGNKI, Moscow, Moscow
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- TP 206 **An Automated Technique for Multiresidue Analysis of Pesticides in Agricultural Samples;** Rudolf Addink¹; Hamid R Shirkhan¹; ¹Toxic Report, Watertown, MA
- TP 207 **Multi-residue Veterinary Drug Analysis of >200 Compounds using MRM Spectrum Mode by LC-MS/MS;** David Baker¹; Laetitia Fages²; Eric Capodanno²; Neil Loftus¹; Simon Ashton¹; ¹Shimadzu, Manchester, UK; ²Phytocontrol, Nîmes, France
- TP 208 **Multi-Residue Pesticide Analysis in Food Matrices using HPLC/MS/MS;** Theresa Sosienski¹; Dan-Hui Dorothy Yang¹; Joan Stevens²; Patrick Jeanville¹; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies, Inc., Wilmington, DE
- TP 209 **Matrix-effect Free Quantitative Analysis using Nanoflow Liquid Chromatography High Resolution Mass Spectrometry;** David Moreno-González¹; Jaime Alcantara-Durán¹; Antonio Molina-Díaz¹; Juan F. García-Reyes¹; ¹University of Jaen, Jaen, Andalusia
- TP 210 **Solid Phase Extraction and SFC-MS/MS Method for Analysis of Aflatoxins M1, M2, B1, B2, G1 and G2 in Milk Powders;** Jun Xiang Lee¹; Yin Ling Chew¹; Zhaoqi Zhan¹; Jie Xing¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore
- TP 211 **Development of Sensitive and Selective Methods for Identification of Marine Toxins by Liquid Chromatography Tandem Mass Spectrometry;** Manami Kobayashi¹; Junichi Masuda¹; Yoshihiro Hayakawa²; ¹Shimadzu Corporation, Hadano-city, Japan; ²Shimadzu Corporation, Kyoto-city, Japan
- TP 212 **Determination of Chemical Contaminants in Indian Prawns by Fast GC-MS/MS using Modified QuEChERS as an Extraction Method;** Durvesh Sawant¹; Prashant Hase¹; Jitendra Kelkar¹; Ankush Bhone¹; Sanket Chiplunkar¹; Dheeraj Handique¹; Nitish Suryawanshi¹; Ajit Datar¹; Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- TP 213 **A Streamlined Multi-Residue Method for Quantitation and Confirmation of Selected Veterinary Drug Residues in Milk by High-Resolution Mass Spectrometry;** Kithsiri B Herath¹; Hernando Escobar¹; Lauren A. Girard¹; Sherri B. Turnipseed²; Philip J. Kijak¹; Hiranthi Jayasuriya¹; ¹Center for Veterinary Medicine/FDA, Laurel, MD; ²U.S. Food and Drug Administration, Denver, CO
- TP 214 **DART-FTMS Detection of Melamine-Lactose Adducts and Condensation Products in Experimentally Adulterated Milk Powders;** Peter Scholl¹; Luke K Ackerman¹; Joseph H LaPointe²; Zhuohong Xie³; Jeffrey C Moore³; ¹US FDA, College Park, MD; ²IonSense Inc., Saugus, MA; ³U.S. Pharmacopeia, Rockville, MD
- TP 215 **Development of Compounds Identification by Using Various Chromatography and Multiple Mass Spectrometry in Food Adulteration;** Chun-Ye Sun¹; Shao-Zhen Wang¹; Heng-Tao Dong¹; ¹Agilent Technology, Inc., Shanghai, China
- TP 216 **Glyco-signature for Human Saliva: Human Saliva can be Determined by Highly Fucosylated Glycans;** Hantae Moon^{1,2}; Bum Jin Kim^{1,2}; Hyun Joo An^{1,2}; ¹Chungnam National University, Daejeon, South Korea; ²Asia Glycomics Reference Site, Chungnam National University, South Korea
- TP 217 **Multivariate Data Analysis in the Interpretation of GC-MS fire Debris Results;** Marco Pazzi¹; Laura Pacifici¹; Eugenio Alladio^{1,2}; Fabrizio Malaspina³; Marco Vincenti^{1,2}; ¹Dipartimento di Chimica, Università degli Studi di Torino, Torino, Italy; ²Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole 10/1, 10043 Orbassano (Torino), Italy; ³Corpo Nazionale Vigili del Fuoco - Comando di Torino, Unità di Intervento Nucleare Biologico Chimico Radiologico, Torino, Italy
- TP 218 **Quantitation of THC and Metabolites in Whole Blood By LC-MS/MS For Per Se Law Testing;** Diana Tran^{1,2}; Xiang He²; Tracy Blethen²; Kevin Kopp³; Matt Kopp³; Alexandre Wang²; Hua-Fen Liu²; ¹Redwood City, CA; ²SCIEX, Redwood City, CA; ³UTAK Laboratories Inc, Valencia, CA
- TP 219 **Multi-targeted Screening Procedures to Detect Prohibited Substances by LC-MS-based Techniques in Doping Control: Evaluation of Different Extraction Protocols;** Fabio Comunità¹; Xavier de la Torre¹; Monica Mazzarino¹; Francesco Bottrè^{1,2}; ¹Antidoping laboratory of Rome, Rome, Italy; ²Università Degli Studi di Roma "Sapienza", Rome, Italy
- TP 220 **Doping Control Analysis of Two Major JWH-250 Urinary Metabolites, JWH-250 4-OH-pentyl and JWH-250 5-OH-pentyl, in Equine urine by LC-MS/MS;** Youwen You^{1,2}; Rachel M. Proctor^{1,2}; Eric D. Vasilko^{1,2}; Mary A. Robinson^{1,2}; ¹University of Pennsylvania, Kennett Square, PA; ²PA Equine Toxicology & Research Laboratory, West Chester, PA
- TP 221 **Drug Analysis in Urine by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS);** Hiroko Abe¹; Chikako Takei²; Yasuo Shida²; Motoshi Sakakura³; Teruhisa Shiota³; Kayako Suga⁴; Daisuke Yajima¹; Hirotaro Iwase^{1,5}; ¹University of Chiba, Chiba, Japan; ²BioChromato, Inc., Fujisawa, Japan; ³AMR Inc., Meguro-ku, Japan; ⁴SCIEX, Shinagawa, Japan; ⁵University of Tokyo, Bunkyo, Japan
- TP 222 **Strategies for Multiple-Target Screening using LC-MS/MS with Merged Spectrum Database for Forensic Toxicology;** Toshikazu Minohata¹; Yutaro Yamamura¹; ¹Shimadzu Corporation, Kyoto, Japan
- TP 223 **A Novel Liquid Chromatography Tandem Mass Spectrometry Method Detection of Deinagkistrodon acutus venom in vivo;** Hangqi Li¹; Jia Lin¹; Chao Zhang²; Peibin Qin²; Huaidong Yu²; ¹Institute of Forensic Science of Fujian Public Security Department, Fuzhou, China; ²SCIEX Asia Pacific Application Support Center, Beijing, China
- TP 224 **Rapid Analysis of Protein Toxins using Hot Acid Digestion and MALDI-TOF with Post-Source Decay;** Dapeng Chen¹; Wayne A. Bryden²; Catherine Fenselau¹; ¹Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; ²Zeteo Tech LLC, Ellicott City, MD
- TP 225 **The Utility and Legality of Using Portable, Ambient Sampling Mass Spectrometers in Traffic Stops;** Alessandra M. Bruno¹; Scott Cleary¹; Michael C. Gizzi²; Christopher C. Mulligan¹; ¹Department of Chemistry, Illinois State University, Normal, IL; ²Department of Criminal Justice Sciences, Illinois State University, Normal, IL
- TP 226 **The Advantages of Direct Analysis of Morphine and its Metabolites with Related Compounds in Urine by LC-MS/MS;** Justin Steimling¹; Frances Carroll¹; Susan Steinike¹; ¹Restek Corporation, Bellefonte, PA
- TP 227 **A New Algorithm for Identifying Emerging Designer**



TUESDAY POSTERS

- Drugs – A Case Study using Fentanyl;** Arun S. Moorthy¹; William E. Wallace¹; Anthony J. Kearsley¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹National Institute of Standards & Technology, NIST, Gaithersburg, MD
- TP 228 **Soft-Landed Metallic Nanoparticles for Mass Spectrometry Imaging of Fingermarks;** Roberto Aguilar¹; Guido F. Verbeck²; ¹University of North Texas, Denton, TX; ²University of North Texas, Denton, TX
- TP 229 **Automated Semi-Quantitative Screening of Benzodiazepines and Designer Benzodiazepines in Human Serum using LC-ion Trap-MS;** Ronja Peter^{1,2}; Maurice Wilde^{2,3}; Jürgen Kempf²; ¹Offenburg University of Applied Sciences, Offenburg, Germany; ²Institute of Forensic Medicine, Forensic Toxicology, Medical Center - University of Freiburg, Freiburg, Germany; ³Hermann Staudinger Graduate School, University of Freiburg, Freiburg, Germany
- TP 230 **Separation of Isomeric Cannabinoids by High-Resolution Ion Mobility-MS for the Differentiation of Legal and Illegal Marijuana;** Marianne Hädener¹; Marc Gonin²; Michael Kamrath²; Wolfgang Weinmann¹; Michael Groessl³; ¹University of Bern, Bern, Switzerland; ²TOFWERK, Thun, Switzerland; ³University Hospital Bern, Bern, Switzerland
- TP 231 **Development of an Extraction Method for Identification of a Biomarker of Sarin Exposure in Hair;** Ronald Evans¹; Richard J. Lawrence¹; Susan L. Byers²; Christopher E. Byers¹; Paul Demond²; ¹U.S. Army ECBC, APG-EA, MD; ²Excet, Inc., Springfield, VA
- TP 232 **Generic Extraction Method for Screening of 8 Drugs of Abuse in Saliva with a Quick Turnaround Analysis by LDTD-MS/MS;** Sylvain Letarte¹; Jonathan Rochon²; Serge Auger³; Jean Lacoursiere³; Pierre Picard³; ¹Phytionix Instruments, Boisbriand, QC; ²Université Laval, Quebec, QC; ³Phytionix Technologies, Quebec, QC
- TP 233 **Characterizing Exogenous Marijuana Components in Breath using a Novel Collection Device and Gas Chromatography/Mass Spectrometry;** Bruce A. Benner¹; D'Nisha D. Hamblin¹; Michele M. Schantz¹; William A. MacCrehan¹; José R. Almirall²; ¹NIST, Gaithersburg, MD; ²Florida International University, Miami, FL
- TP 234 **Comparison between High-resolution Separation and Site-specific-enzymatic Identification of Aspartic Acid and Asparagine Racemization, Isomerization, and Racemization in Eye Lens Crystallins;** Kaitlin Long¹; Mehdi Moini²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
- TP 235 **Quick Identification of Uranium Compounds using Thermal Ionization Time-of-Flight Mass Spectrometry;** Dongfa Guo¹; Zengwei Fan¹; Guifang Liu¹; Yuang Liu¹; Shengkai Xie¹; Jianyong Cui¹; ¹Beijing Research Institute of Uranium Geology, Beijing, China
- TP 236 **Optimization of Peptide Generation from Human Hair for Proteomic Analysis;** Zachary C. Goecker¹; Glendon J. Parker¹; Robert H. Rice¹; Michelle R. Salemi²; Brett S. Phinney²; ¹University of California, Davis, Davis, CA; ²Proteomics Core Facility, Genome Center, University of California, Davis, Davis, CA
- TP 237 **"Fowl" Odors: Identification of Blow Fly Attraction Cues in Decomposing Chicken Livers;** Justine E. Giffen¹; Jennifer Y. Rosati²; Rabi A. Musah¹; ¹University at Albany-SUNY, Albany, NY; ²John Jay College of Criminal Justice, New York, NY
- TP 238 **Bouquet of Death: Determination of Carrion Flower Blowfly Attractants by Ambient Mass Spectrometry;** Rabi Musah¹; Justine E. Giffen¹; Jennifer Y. Rosati²; Kristen Fowble¹; ¹University at Albany-SUNY, Albany, NY; ²John Jay College of Criminal Justice, New York, NY
- TP 239 **Comparison of Screening and Quantitative LC-MS-**
- MS Analysis of Drugs and Their Metabolites on Triple Quadrupole and Quadrupole Orbitrap Mass Spectrometers**; Rory M. Doyle¹; Kevin McHale¹; ¹Thermo Fisher Scientific, Somerset, NJ
- TP 240 **LC-MSMS Analysis of Serum Samples for the Detection and Quantification of Corticosteroids in Equine Sport;** Erin Crum¹; Jeshurun Benavides¹; Nina Salazar¹; Richard Sams¹; ¹LGC Ltd US, Lexington, KY
- TP 241 **Development of Succinylcholine Chloride in Biologic Extracts using Liquid Chromatography-Tandem Mass Spectrometry;** Dai-Yong Huang¹; Jun-Gang Lu²; Cai-Yong Lin²; Zhi-quan Yuan²; Shan-An Chan³; ¹Agilent Technologies Ltd. Hong Kong, Hong Kong, Hong Kong; ²Agilent Technologies (China), Guangzhou, China; ³Agilent Technologies Inc., Taipei, Taiwan
- FUNDAMENTALS: ION SPECTROSCOPY**
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- TP 242 **Infrared Predissociation Spectroscopy Inside a Cryogenic Mass-Selective Trap;** Matthew Bell¹; Nicolas C. Polfer¹; ¹University of Florida, Department of Chemistry, Gainesville, FL
- TP 243 **IRPD Spectroscopy of Metal Cationized Ions Generated by MADLI Source: What is New?;** Xianglei Kong; Nankai University, Tianjin
- TP 244 **Exploring Gas-Phase Structures and Properties of DNA-based Cation-Radicals with UV Action Spectra and Excited State Computations;** Andy Dang¹; Joseph A. Korn¹; Frantisek Turecek¹; ¹University of Washington, Seattle, WA
- TP 245 **Gas-Phase Conformations and N-Glycosidic Bond Stabilities of Sodium Caionized Cytosine Nucleosides: Solution Conformation of [Cyd+Na]⁺ is Preserved upon ESI;** Yanlong Zhu¹; Lucas A. Hamlow¹; Chenchen He¹; Harrison A. Roy¹; Nathan Cunningham¹; Musleh Munshi²; Giel Berden²; Jos Oomens²; Mary T. Rodgers¹; ¹Wayne State University, Detroit, MI; ²FELIX Facility, Radboud University, Netherlands
- TP 246 **Cryogenic Spectroscopy of the Protonated Serine Octamer;** Valeriu Scutelnic¹; Marta Perez¹; Aurelien Gregor¹; Ursula Röthlisberger¹; Thomas R. Rizzo¹; ¹EPFL, Lausanne, Switzerland
- TP 247 **A Cryogenic Linear Ion Trap for Fluorescence Spectroscopy;** Alessandra Ferzoco¹; Vaishnavi Rajagopal¹; ¹Rowland Institute at Harvard, Cambridge, MA
- TP 248 **Gas-phase Infrared Spectroscopy of Proteins and Protein Assemblies;** Stephan Warnke¹; Jongcheol Seo²; Waldemar Hoffmann²; Michael T. Bowers³; Kevin Pagel⁴; Gert von Helden²; ¹École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Berlin; ³University of California Santa Barbara, Santa Barbara, CA; ⁴Freie Universität Berlin, Berlin, Germany
- TP 249 **Characterizing Peptide-Hairpin Loops via Cold Ion Spectroscopy of Model Compounds;** John Thomas Lawler¹; Christopher P. Harriall¹; Andrew DeBlase¹; Scott A. McLuckey¹; Timothy S. Zwier¹; ¹Purdue University, West Lafayette, Indiana
- TP 250 **Structural and Energetic Characterization of Modified Nucleosides on a Bruker amaZon ETD Quadrupole Ion Trap Mass Spectrometer;** Lucas Hamlow¹; Yanlong Zhu¹; Zachary Devereaux¹; Mary T. Rodgers¹; ¹Wayne State University, Detroit, MI
- TP 251 **Effect of Ion Cooling in Ion Trap RF Fields;** Sergey Poteshin¹; Anna Burykina¹; Nikita Komar¹; ¹National Research Nuclear University MEPhI, Moscow, Moscow
- TP 252 **Long Distance Ion-Water Interactions in Aqueous Sulfate Nanodrops Orient Surface Water Molecules up to Tropospheric Temperatures;** Matthew J. DiTucci¹; Christiane N. Stachl¹; Evan R. Williams¹; ¹University of



- California, Berkeley, Berkeley, CA
- TP 253 **Probing Conformational Isomerization and Relative Abundances between Major Conformers of 10K Gas Phase [YAP(D-Pro)AA+H]⁺ Ions using IR-UV Double Resonance;** Christopher Harrilal¹; Andrew DeBlase¹; Joshua Fischer¹; John T Lawler¹; Nicole L Burke¹; Timothy S Zwier¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette
- TP 254 **Photodissociation Action Spectroscopy of Protonated N-containing Aromatic Ions: Can We Predict Photodissociation Pathways?**; James Bezzina¹; Stephen J Blanksby²; Adam J Trevitt¹; ¹University of Wollongong, Wollongong, NSW; ²Queensland University of Technology, Brisbane, Australia
- TP 255 **Reactivity and Kinetics of Ortho-substituted Phenylnitrenes;** Christopher Haskins¹; Paul G Wenthold¹; ¹Purdue University, West Lafayette, Indiana
- TP 256 **Energetics and Mechanism of CO₂ Activation by Gadolinium Cation (Gd⁺);** Maria Demireva¹; Peter B. Armentrout¹; ¹University of Utah, Salt Lake City, UT
- TP 257 **Investigation on the Unimolecular and Collisional-Activated Fragmentation Mechanisms of diethyltoluidines with Isotopic Labelling Experiments;** Sarah Seulen¹; Jurgen Grotemeyer¹; ¹Christian Albrechts University at Kiel, Institute for Physical Chemistry, Kiel, Germany
- TP 258 **Fragmentation Mechanisms of Azo Dye Molecules Containing Diethylamino Groups – Thermodynamic and Kinetic Considerations;** Martin Clemen¹; Jurgen Grotemeyer¹; ¹Christian Albrechts University at Kiel, Institute for Physical Chemistry, Kiel, Germany
- TP 259 **The Structure of FeIII-Aerobactin Complexes: an Empirical and Theoretical Study;** Daryl Giblin¹; Jan R Crowley²; Hung Tran²; Michael L. Gross³; Jeffrey P. Henderson²; ¹Washington University, St Louis, MO; ²Department of Internal Medicine, Washington University School of Medicine, St. Louis, MO; ³Department of Chemistry, Washington University, St. Louis, MO
- TP 260 **Anionic Carbohydrate Gas-Phase Chemistry: Gelling Experimental and Theoretical Methods;** Jordan M Rabus¹; Benjamin J Bythell¹; ¹University of Missouri-St. Louis, St. Louis, MO
- TP 261 **Radical-Mediated Reactions of Peptide Radical Cations: Isomerization versus Dissociation;** Xiaoyan Mu¹; Justin Kai-Chi Lau^{2,3}; Alan C. Hopkinson²; Ivan K. Chu¹; ¹University of Hong Kong, Hong Kong; ²York University, Toronto, ON; ³University of Windsor, Windsor, ON
- TP 262 **Fragmentation Reactions of a7 Ions from Singly Protonated Model Heptapeptides Containing Glutamine Residue;** Ahmet Emin Atik¹; Alex. G. Harrison²; Talat Yalcin¹; ¹IYTE, Urla-Izmir; ²University of Toronto, Toronto, ON
- TP 263 **Gas-Phase Acidities and Conformations of Oligopeptide Epimers with D- and L-Cysteine;** Yuntao Zhang¹; Zachary Buen¹; Jianhua Ren¹; ¹University of the Pacific, Stockton, CA
- TP 264 **Investigation of the Self-Assembly Mechanism of Sandwich-Type Polyoxometalates using Mass spectrometry and X-ray crystallography;** Jie Cao¹; Chang-Wen Hu¹; Lin-Yuan Fan¹; ¹Beijing Institute of Technology, Beijing, China
- TP 265 **Fragmentation and H/D Exchange Studies of Tetrapeptides Containing Lysine Homologues;** Melanie A Berger¹; Zachariah I. Hasan¹; Anna Do¹; Danielle A. Long¹; Anwar Radwan¹; John Poutsma¹; ¹College of William & Mary, Williamsburg, VA
- TP 266 **IRMPD Studies of b2 and b3 Ions From Lysine Analog-Containing Peptides;** Zachary M. Smith¹; Vincent Steinmetz²; Arpad Somogyi³; Vicki H. Wysocki³; John Poutsma¹; ¹College of William & Mary, Williamsburg, VA; ²Université de Paris Sud, Orsay, France; ³Ohio State University, Columbus, OH
- TP 267 **Role of Residual Water Molecules into a Linear Ion**
- Trap Cell on Re-Orientation of Aspartate and Glutamate Anion Dissociations;** Pierre Barbier Saint Hilaire¹; Yves Gimbert²; Anna Warnet¹; Annelaure Damont¹; Marie-Françoise Olivier¹; Benoît Colsch¹; François Fenaille¹; Christophe Junot¹; Jean-Claude Tabet^{1,3}; ¹CEA, iBiTecS, SPI, Laboratoire d'Etude du Métabolisme des Médicaments, MetaboHUB-Paris, Université Paris Saclay, Gif-sur-Yvette cedex, France; ²Université Grenoble Alpes (DCM), CNRS-UJF 5250, BP 38041, Grenoble, France; ³Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France
- TP 268 **An Ion Mobility Database of Metal-Coordinated Peptide Ions: General Structural Effects upon Alkali, Alkaline-earth, or Transition-metal Interaction;** Jonathan Dilger¹; David E Clemmer²; ¹Naval Surface Warfare Center, Crane Division, Crane, IN; ²Indiana University Bloomington, Bloomington, IN
- TP 269 **Size-selective Anion Binding by Cucurbit[5]uril Characterized Using SORI-CID Techniques;** Jiewen Shen¹; David V. Dearden²; ¹Brigham Young University, Provo, UT; ²Brigham Young University, Provo, UT
- GC/MS: INSTRUMENTATION AND APPLICATIONS II**
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- TP 270 **Chemometric Methods for Analysis of Graftage-related Black Tea Aroma Variation by Solid Phase Mirco-extraction and Gas Chromatography-Mass Spectrometry;** Wei Chen¹; Wenwen Wang²; Chengying Ma¹; Junxi Cao¹; Aiqing Miao¹; Shi Pang¹; ¹Tea Research Institute, Guangdong Academy of Agricultural Sciences, Guangzhou, China; ²Agilent Technologies (China), Beijing, China
- TP 271 **Atmospheric Pressure Gas Chromatography/Mass Spectrometry for the Analysis of Organochlorine Pesticides, Polychlorinated Biphenyls and Polybrominated Diphenyl Ethers in Human Serum;** Jing Fang¹; Xiubao Huang¹; Yanhao Zhang¹; Hongzhi Zhao¹; Zongwei Cai¹; ¹State Key Laboratory of Environmental and Analytical Chemistry, Department of Chemistry, Hong Kong Baptist University, Hong Kong, Hong Kong
- TP 272 **Simultaneous Determination of 12 Tobacco Alkaloids in E-liquids for Electronic Cigarettes Using Gas Chromatography - Mass Spectrometry Method;** Shulei Han¹; Yaning Fu¹; Tong Liu¹; Huan Chen¹; Hongwei Hou¹; Qingyuan Hu¹; ¹China National Tobacco Quality Supervision & Test Centre, Zhengzhou, China
- TP 273 **Determination of Fatty Acid Esters of 2- and 3-monochloro-1,2-propanediol (MCPD) and Glycidol in Edible Oil Using GC-Triple Quadrupole Mass Spectrometry;** Samuel Chao Ming Yeo¹; Crystal Hui Xian Yeong¹; Kok Ming Goh²; Chin Pang Tan²; May Yen Ang³; Lai Chin Loo¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; ²Department of Food Technology, Faculty of Food Science and Technology, Universiti Putra Malaysia, 43400 UPM Serdang, Malaysia; ³Shimadzu Malaysia Sdn Bhd, Taman Sains Selangor I, Malaysia
- TP 274 **Quantifying Flavorings in E-cigarette Aerosol as a Function of Power Applied to the Heating Coil;** Nicholas Wallbillich¹; Gary Glish²; ¹UNC, Chapel Hill, NC; ²Professor, Chapel Hill, North Carolina
- TP 275 **Analysis of Cannabidiols found in Cannabis by Thermal Desorption GC/MS;** Ronald Shomo¹; Christopher Baker¹; John manura¹; ¹Scientific Instrument Services, Ringoes, NJ
- TP 276 **Diagnostically Important Ions in Mass Spectra of Silyl, Sulfonyl, Alkoxy carbonyl and Perfluoroacyl Derivatives of Substituted Phenols;** Nino G. Todua¹; Levan A. Megutnishvili²; Anzor I. Mikaia²; ¹NIST / Dakota C., Gaithersburg, MD; ²NIST, Gaithersburg, MD
- TP 277 **Integrated Microextraction, Syringe Headspace, and**



TUESDAY POSTERS

- TP 278 **SPME Characterization of Organic Contamination from Plastic Bags by GC/MS;** Adam J. Patkin¹; Charlie Schmidt¹; ¹PerkinElmer, Shelton, CT
- TP 279 **Off-flavour Analysis in Food Using a Simple and Rapid Solid Phase Microextraction-GC/Triple Quadrupole Mass Spectrometry Method with Dedicated Off-flavour Database;** Samuel Chao Ming Yeo¹; Cynthia Melanie Lahey¹; Lai Chin Loo¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore
- TP 280 **Qualitative Profiling of Co-polymer Polyethylene Terephthalate through Multifunctional Pyrolyzer-GC/MS by various Thermal Treatment Techniques;** Guo Wei Elgin Ting¹; Stephany Olivia²; Chiang Yong Douglas Chong³; Hui Xian Crystal Yeong¹; Lai Chin Loo¹; ¹Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Cintech IV, Singapore Science Park, Singapore; ²Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore; ³Department of Chemistry, Faculty of Science, National University of Singapore, Singapore
- TP 281 **Analysis of Fast Moving Consumer Goods (FMCG) using GCMS with Static and Dynamic Headspace (HS);** Dheeraj Handique¹; Ankush Bhone¹; Prashant Hase¹; Sanket Chiplunkar¹; Durvesh Sawant¹; Nitish Suryawanshi¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- TP 282 **Addressing the Challenges of Short Chained Chlorinated Paraffins Analysis using Orbitrap GC-MS;** Cristian Cojocariu¹; Paul Silcock²; ¹Thermo Fisher Scientific, Runcorn, UK; ²Thermo Fisher Scientific, Runcorn, Cheshire
- TP 283 **Characterization of Perfumes via Tandem Vacuum Ultraviolet Spectroscopy and Mass Spectrometry;** Ian Anthony¹; Adam R. Floyd¹; Christina A. Gaw¹; Matthew R. Brantley¹; Touradj Solouki¹; ¹Baylor University, Waco, Texas
- TP 284 **Fluorine Tagging for Quantification of Krebs Cycle Metabolites using Gas-Chromatography Plasma Assisted Reaction Chemical Ionization Mass Spectrometry;** Michael Dolan¹; Kunyu Zheng²; Steven Peyton³; Amrita Cheema³; Kaveh Jorabchi²; ¹Georgetown University, Washington, DC; ²Georgetown University, Washington, DC; ³Georgetown University Medical School, Washington, DC
- TP 285 **Loss of SO₂ from o-Nitro Substituted Diaryl Sulfides and Related Compounds;** Yufang Zheng¹; Quanlong Pu²; Edward White V²; Stephen E. Stein²; ¹NIST / Dakota C., Gaithersburg, MD; ²NIST, Gaithersburg, MD
- TP 286 **Method for Determining Kinetic Parameters of Chemical Warfare Nerve Agent Decomposition via Pyrolysis GC-MS;** Jeffrey Michael McGuire¹; John C Carpin¹; William T Muse¹; ¹US Army ECBC, Aberdeen Proving Ground, MD
- TP 287 **Analysis of Modified Graphene Oxide nanomaterial using STA/FT-IR/GC-MS;** Xiaoying Yan¹; Zhuo Man²; Xiangdong Zhou²; Jason Weisenseel³; Yong-Ming Xie²; ¹National Center for Nanoscience and Technology, Beijing, China; ²PerkinElmer Management (Shanghai) Co, Shanghai, China; ³PerkinElmer, Shelton, CT
- TP 288 **Analysis of Unknown Contaminants in Interior Air Spray using TGA/FT-IR/GC-MS;** Fei Zhang¹; Zhuo Man²; Xiangdong Zhou²; Desmond Wichems³; Yongming Xie²; ¹Peking University, Beijing, Beijing; ²PerkinElmer Management (Shanghai) Co, Shanghai, China; ³PerkinElmer Inc., San Jose, CA
- TP 289 **Evaluation of select-eV, two-dimensional-GC and Large Volume Injection on the Limits of Detection and Quantification of Cannabinoids in Hair Samples;** Emma Beasley¹; Geraint Morgan²; Tom Bassindale¹; ¹Sheffield Hallam University, Sheffield, UK; ²The Open University, Milton Keynes, UK
- TP 290 **Headspace Solid Phase Micro-Extraction (HS-SPME) of Volatile Compounds Encapsulated in Flash Frozen Coffee Extracts;** Mary Elizabeth Gimon-Kinsel¹; Jackson Frazier Wood¹; ¹Southern Illinois University, Carbondale, IL
- TP 291 **Identification of Salivary Metabolomics Biomarkers of Chronic Kidney Disease and Their Association with Periodontitis;** Levy Alves^{1,2,3,4}; Rafael Celestino Souza³; Taciana Mara Couto da Silva Mara Couto da Silva³; Meriellen Dias^{2,5}; Deise Garrido^{3,5}; maria anita mendes^{2,5}; Ana Lidia Ciamponi^{3,5}; ¹Guarulhos University, São Paulo, SP; ²Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil; ³Dental School of USP, São Paulo, Brazil; ⁴Paulista University, São Paulo, Brazil; ⁵Universidade de São Paulo - USP, Sao Paulo, South America
- TP 292 **Evaluation of a High-Sensitivity GC-MS/MS in the Analysis of Pesticide Residues in Complex Samples: Cost Savings and Other Benefits;** Katerina Mastovska¹; Lukas Vacklavik²; Melissa Churley³; Thomas P. Doherty³; ¹Covance, Madison, WI; ²Covance, Harrogate, UK; ³Agilent Technologies, Inc., Santa Clara, CA
- TP 293 **Applying Pyrolysis GC/MS to the Characterization of Agricultural Formulations;** Todd Kajdan; Dow AgroSciences, Indianapolis, IN
- TP 294 **GCMS and NMR Based Chemometrics of Distillates;** Mary Jean Riches¹; Kaylen Obray¹; Karolien Deneff¹; Claudia Boot¹; Chris Rithner¹; ¹Colorado State University, Fort Collins, CO
- TP 295 **Determination of Retention Indices of Organic Compounds in Comprehensive Two-Dimensional Gas Chromatography-Mass Spectrometry (GCxGC-MS);** Dmitrii Mazur¹; Olga Polyakova¹; Albert Lebedev¹; ¹M.V. Lomonosov Moscow State University, Moscow, Russia
- TP 296 **Fast Screening and Quantitation of Perfluorinated Sources from Textiles Using Gas Chromatography Chemical Ionization Mass Spectrometry;** Hui Xian Crystal Yeong¹; Stephany Olivia²; Lai Chin Loo¹; ¹Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Cintech IV, Singapore Science Park 1, Singapore 118264, Singapore; ²Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore
- TP 297 **Fast and Accurate Quantitation of Perfluorinated Sources from Textiles Using Gas Chromatography-Triple Quadrupole Mass Spectrometry;** Hui Xian Crystal Yeong¹; Stephany Olivia²; Cynthia Melanie Lahey¹; Guo Wei Elgin Ting¹; Lai Chin Loo¹; ¹Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Cintech IV, Singapore Science Park 1, Singapore 118264, Singapore, Singapore; ²Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore
- TP 298 **Determination of Cannabinoids from a Surrogate Hops Matrix Using Multiple Reaction Monitoring Gas Chromatography – Triple Quadrupole – Mass Spectrometry;** Allegra Leghissa¹; Kevin A. Schug²; ¹University Of Texas, Arlington, Arlington, TX; ²University of Texas, Arlington, Arlington, TX
- TP 299 **GLYCOPROTEINS I**
298 - 324
A Method for the Quantitative Monitoring of Site-Specific Glycosylation of Proteins in Large Sample Set Analysis; Elisha Goonatileke¹; Jincui Huang¹; Lauren Dimapasoc Wu¹; Gege Xu¹; Carlito B Lebrilla¹; ¹University of California, Davis, Davis, CA
- TP 299 **Site-Specific Fucosylation Analysis of Glycoproteins**



- from Aggressive Prostate Cancer Cells Using Affinity Enrichments of Intact Glycopeptides Followed by Mass Spectrometry; Jianliang Zhou¹; Weiming Yang¹; Yingwei Hu¹; Naseruddin Hoti¹; Punit Shah¹; Hui Zhang¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD
- TP 300 **Comparison of Site-Specific N-Glycoproteins between Human and Mouse Plasma Using LC-MS/MS and Database Search**; Juyeon Lee^{1,2}; Hyun Kyoung Lee^{1,3}; Gun Wook Park¹; Kun Cho^{1,2}; Jeong Gu Kang²; Yong-Sam Kim²; Jeong-Heon Ko²; Jin Young Kim¹; Jong Shin Yoo¹; ¹Korea Basic Science Institute, 162 YeonGuDanji-Ro, Ochang-eup, Cheongwon-gu, Cheongju, South Korea; ²Korea Institute of Bioscience and Biotechnology, Daejeon, South Korea; ³Graduate School of Analytical Science and Technology, Daejeon, South Korea
- TP 301 **Glycosylation Analysis of Spike Protein from Infectious Bronchitis Viruses with Different Tissue Binding Properties**; Lisa Parsons¹; Kim Bouwman²; Helene Verheije²; John F Cipollo¹; ¹FDA, Silver Spring, MD; ²Utrecht University, Utrecht, Netherlands
- TP 302 **Glycoproteomics Analysis to Examine the Role of Chlamydial Protease-Like Activity Factor**; Christa Feasley¹; Fred Zinnel²; Julian Saba³; Stuart McCrister⁴; Garrett Westmacott⁴; Grant McClarty⁴; Chris Grant⁴; ¹Thermo Fisher Scientific, West Palm Beach, Florida; ²Thermo Fisher Scientific, Somerset, NJ; ³Thermo Fisher Scientific, Mississauga, Ontario; ⁴National Microbiology Laboratory, Public Health Agency of Canada, Winnipeg, MB
- TP 303 **Glycoproteomic Analysis of Temozoleamide-Resistant Glioma Cells by MALDI-TOF/TOF MS and nano-HPLC-QTOF-MS/MS**; Milan Teraiya¹; Emy Komatsu¹; Jenna Noordenbos²; Helene Perreault³; Vincent C Chen²; ¹University of Manitoba, Winnipeg, MB; ²Brandon University, Department of Chemistry, Brandon, MB; ³University of Manitoba, Winnipeg, MB
- TP 304 **Global Analysis of Secreted N-Glycoproteins in MCF7 Cells Using Click Chemistry-Based Enrichment and Mass Spectrometry**; Fangxu Sun¹; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 305 **Quantitative Analysis of N- and O- Glycans from Cerebrospinal Fluid in Alzheimer's Disease Patients**; Byeong G. Cho¹; Aiyng Yu¹; Lucas Veillon¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- TP 306 **Site-Specific Characterization and Quantitation of N-Glycoproteins in Breast Cancer Cells Using DiLeu Isobaric Tags Enabled by Electron-Transfer/Higher-Energy Collision Dissociation (ETHCD)**; Zhengwei Chen¹; Qing Yu¹; Ling Hao¹; Fabao Liu¹; Jill Johnson¹; Zichuan Tian¹; Wei Xu¹; Lingjun Li¹; ¹University of Wisconsin Madison, Madison, WI
- TP 307 **Systematic Investigation of Glycan Maturity on Human Cell Surface Glycoproteins**; Suttipong Suttapitugsakul¹; Johanna Smeekens¹; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 308 **Mass Spectrometry-Based Characterization of Recombinant Human Immunodeficiency Virus Type 1 (HIV-1) Envelope (Env) Glycoprotein**; Vaneet Kumar Sharma; International AIDS Vaccine Initiative (IAVI), New York, NY
- TP 309 **An Insight into Glyco-microheterogeneity of Plasma von Willebrand Factor (vWF) by MS Spectrometry**; Ebtesam Gashash^{1,2}; Arya Aloor¹; He Zhu¹; Cong Xiao¹; Ding Liu¹; Jing Song¹; Cheng Ma¹; Weidong Xiao³; Peng Wang¹; ¹GSU, Atlanta, GA; ²Albaha University, Baljurashi, Saudi Arabia; ³Sol Sherry Thrombosis Research Center, Temple University, Philadelphia, PA 19140
- TP 310 **A Novel Method Combining Enzymatic and Chemical Reactions to Identify Glycoproteins with the Tn Antigen**; Jiangnan Zheng¹; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 311 **Effects of Illiciting Immune Response in Rabbits on IgG N-Glycans**; Tyler Fletcher¹; Ron Orlando¹; ¹University of Georgia, Athens, GA
- TP 312 **Glycan Heterogeneity Differentiation Using Lectin-Based SDC Separation and Glycopeptide level SDC Separation**; Wonryeon Cho; Wonkwang University, Iksan, Jeonbuk
- TP 313 **Assisting the Characterization of IgG Glycosylation with a Hydrophilic Interaction Liquid Chromatography Retention Model for Glycopeptides**; Emily Betchy¹; Barry Boyes²; Ron Orlando¹; ¹CCRC, University of Georgia, Athens, GA; ²Advanced Materials Technology, Wilmington, DE
- TP 314 **Characterization of Glycan Structures of Zika Virus**; Zhichao Zhang¹; Christopher Brown²; Yixiang zhang²; David E Clemmer²; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- TP 315 **Comparative Glycomic Approaches for Assessment of Glycosylation in a Therapeutic Glycoprotein**; Nayoung Yun^{1,2}; Nari Seo^{2,3}; Unyong Kim²; Myung Jin Oh^{2,3}; Hyun Joo An^{2,3}; ¹Chungnam National University, Daejeon, Chungcheongnam; ²Asia Glycomics Reference Site, Daejeon, South Korea; ³Chungnam National University, Daejeon, South Korea
- TP 316 **Workflows for the Identification and Relative Quantitation of Glycan Variants**; Stephen Madden¹; Aaron Boice¹; Aditi Koul¹; Caroline S. Chu¹; ¹Agilent Technologies, Inc., Santa Clara, CA
- TP 317 **Identification of Glycoprotein Biomarkers for Hepatocellular Carcinoma**; Cristina Di Poto¹; Minkun Wang¹; Shan Su¹; Junfeng Ma¹; Habtom W. Ressim¹; ¹Georgetown University, Lombardi Cancer Center, Washington, DC
- TP 318 **Glycoproteomic Identification and Quantification of Human Plasma with IQ-GPA and Database Search**; Gun Wook Park¹; Jin Young Kim¹; Ju Yeon Lee¹; Heeyoun Hwang¹; Hyun Kyoung Lee¹; Eun Sun Ji¹; Kwang Hoe Kim^{1,2}; Hoi Keun Jeong^{1,2}; Ki Na Yun^{1,3}; Yong-Sam Kim⁴; Jeong-Heon Ko⁴; Jong Shin Yoo^{1,2}; ¹Biomedical Omics Group, Korea Basic Science Institute, Cheongju-si, South Korea; ²Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; ³Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, South Korea; ⁴Cancer Biomarkers Development Research Center, Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea
- TP 319 **Global and Site-Specific Analysis Reveals Unexpected and Extensive Protein S-GlcNAcylation in Human Cells**; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Tech, Atlanta, GA
- TP 320 **New Analytical Platform to Explore Haptoglobin Glycosylation Using Intact Glycoprotein**; Unyong Kim^{1,2}; Hantae Moon^{1,2}; Sung Hyun Lee³; Myung Jin Oh^{1,2}; Jua Lee^{1,2}; Seung Hyup Jeong^{1,2}; Hyun Joo An^{1,2}; ¹Asia Glycomics Reference Site, Chungnam National University, South Korea; ²Chung Nam Univ., Daejeon; ³Glycan Inc., Seongnam-si, South Korea
- TP 321 **Mass Spectrometry Analysis of Platelet Glycome Using Intact Glycopeptides Analysis Approach**; Punit Shah¹; Hui Zhang¹; ¹Johns Hopkins University, Baltimore, MD
- TP 322 **An O-Glycosylated Archaeal Flagellin Extensively Adorned with Two Unusual Saccharides**; Hong Hanh Nguyen¹; Nicole Poweleit¹; Deborah Leon²; Catherine E. Costello²; Joseph A Loo¹; Robert P. Gunsalus¹; Rachel R. Ogorzalek Loo¹; ¹UCLA, Los Angeles, California; ²Boston University, Boston, MA
- TP 323 **Mapping Site-Specific N-Glycosylation of B-Cell Receptor in B-Cell Lymphomas**; Kuan-Ting Pan¹; Carmen Doebele²; Kay-Hooi Khoo³; Thomas Oellerich^{4,5}; Henning Urlaub^{1,7}; ¹Bioanalytical Mass Spectrometry, MPI for Biophysical Chemistry, Goettingen, Germany; ²Department of Hematology/Oncology, Johann Wolfgang



TUESDAY POSTERS

- Goethe University, Frankfurt am Main, Germany; ³Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; ⁴Department of Hematology/Oncology, Johann Wolfgang Goethe University, Frankfurt am Main, Germany; ⁵German Cancer Research Center (DKFZ), Heidelberg, Germany; ⁶Department of Haematology, University of Cambridge, Cambridge, UK; ⁷Bioanalytics, Department of Clinical Chemistry, University Medical Center Goettingen, Goettingen, Germany
- TP 324 **Site-Specific and Structural Analysis of Protein O-Mannosylation in *Saccharomyces cerevisiae***; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- IMAGING MS: SMALL MOLECULES**
325 - 350
- TP 325 **Imaging Mass Spectrometry of Image-Guided Drug Delivery (IGDD) in Thermochemical Ablation**; Chunxiao Guo¹; Dodge Baluya¹; Rick Layman¹; Erik Cressman¹; ¹MD Anderson, Houston, TX
- TP 326 **Visualizing Chemical Communication Governing Metastasis of Ovarian Cancer with Imaging Mass Spectrometry**; Katherine Zink¹; Joanna E Burdette²; Matthew Dean²; Laura M Sanchez²; ¹, Chicago, IL; ²University of Illinois at Chicago, Chicago, Illinois
- TP 327 **Feasibility Studies in Imaging Mass Spectrometry for Evaluating Thermoembolization, a New Interventional Oncologic Technique**; Chunxiao Guo¹; Dodge Baluya¹; Rick Layman¹; Erik Cressman¹; ¹MD Anderson, Houston, TX
- TP 328 **Liquid Chromatography-Mass Spectrometry-Based Metabolomics and Lipidomics Reveal Toxicological Mechanism of Bisphenol F in Breast Cancer Xenografts**; Chao Zhao^{1,2}; Peisi Xie³; Yuanyuan Song¹; Ti Yang¹; Zhi Tang¹; Hailin Wang²; Zongwei Cai¹; ¹State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong SAR, China; ²State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China; ³Ministry of Education Key Laboratory of Analysis and Detection Technology for Food Safety, Fuzhou University, Fuzhou, China
- TP 329 **Multiscale Mass Spectrometry Imaging of Colorectal Cancers by MALDI, DESI and SIMS**; Rory T Steven¹; Adam J Taylor¹; Spencer A Thomas¹; Alan M Race¹; Gregory Hamm²; Nicole Strittmatter²; Rasmus Havelund¹; Renata F Soares³; Andrew D Campbell⁴; Owen J Sansom⁴; Richard J. A. Goodwin⁵; Zoltan Takats³; Josephine Bunch¹; ¹National Physical Laboratory, Teddington, UK; ²AstraZeneca R&D, Cambridge, UK; ³Imperial College London, London, London; ⁴Beatson Institute for Cancer Research, Bearsden, UK; ⁵Astrazeneca, Cambridge, UK
- TP 330 **Mass Spectrometric Analysis of Endogenous Small Molecules and Chemotherapeutic Doxorubicin in a Three-Dimensional Cell Culture Model of Osteosarcoma**; Ieva Palubeckaite¹; Neil Cross¹; Christine Le Maitre¹; David Smith¹; Chris Sammon¹; Malcolm Clench¹; ¹Sheffield Hallam University, Sheffield, UK
- TP 331 **Technical Challenges of Mass Spectrometry Imaging of Doxorubicin Localization in Rat Liver Treated with Drug-Eluting Beads**; Dodge Baluya¹; Andrea Cortes¹; Hideyuki Nishiofuku¹; Rony Avritscher¹; Erik Cressman²; ¹MD Anderson Cancer Center, Houston, TX; ²MD Anderson, Houston, TX
- TP 332 **Gold Nanoparticles as MALDI MSI Matrix for Imatinib Distribution and Quantitation Analysis Inside Tumor Tissues**; Silvia Giordano¹; Lavinia Morosi¹; Francesca Falcetta¹; Mridula Prasad²; Ilaria Fusco Nerini¹; Simonetta Andrea Licandro¹; Roberta Frapolli¹; Paolo Ubezio¹; Maurizio D'Incalci¹; Massimo Zucchetti¹; Pietro Franceschi²; Sonja Visentin³; Enrico Davoli¹; ¹Mario Negri Institute, Milano; ²Fondazione E.Mach, San Michele all'Adige, Italy; ³University of Torino, Turin, Italy
- TP 333 **Mapping the Brain Neurotransmitter Network with MALDI MS Imaging**; Mohammadreza Shariatgorji¹; Luke Odell¹; Anna Nilsson¹; Elva Fridjonsdottir¹; Luay Katan¹; Jonas Sävmarker¹; Matthias Witt²; Per Svenningsson³; Per E. Andren¹; ¹Uppsala University, Uppsala, SE; ²Bruker Daltonics, Bremen, Germany; ³Karolinska Institutet, Stockholm, Sweden
- TP 334 **Matrix Assisted Laser Desorption Ionization Imaging Mass Spectrometry of Human Osteoarthritis Cartilage Reveals the Intra-Tissue Metabolic Heterogeneity**; Maxime Eveque-Mourroux^{1,2,3}; Pieter Emans²; Tim Welting²; Annelies Boonen³; Ron Heeren¹; Berta Cillero-Pastor¹; ¹Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; ²Maastricht University Medical Center, Department of Orthopedic Surgery, Maastricht, Netherlands; ³Maastricht University Medical Center, Caphri Research institute, Maastricht, Netherlands
- TP 335 **Visualizing NMF Distribution across the Human Face by 2D-DESI MS Imaging of Tape-Stripped Stratum Corneum**; Keishi Kihara¹; Akira Motoyama¹; ¹Shiseido Co., LTD., Yokohama, Kanagawa
- TP 336 ***Pseudomonas aeruginosa* Shifts its Specialized Metabolism in Response to Biofilm Inhibitors**; Alanna Condren¹; Laura M. Sanchez¹; ¹University of Illinois, Chicago, Illinois
- TP 337 **Analyzing Liposomal Drug Delivery Systems in Three-Dimensional Cell Culture Models Using MALDI-Imaging Mass Spectrometry and Fluorescence Microscopy**; Jessica K. Lukowski¹; Eric M. Weaver²; Amanda B. Hummon²; ¹, Notre Dame, IN; ²University of Notre Dame, Notre Dame, IN
- TP 338 **MALDI Imaging of Lipase Activity on Textile Surfaces**; Jonatan Hall-Andersen¹; Svend G. Kaasgaard²; Christian Janfelt¹; ¹University of Copenhagen, Copenhagen, Denmark; ²Novozymes A/S, Bagsvaerd, Denmark
- TP 339 **Demonstrating the Applicability of DESI Imaging Coupled with Ion Mobility for Mapping Cosmetic Ingredients on Tape Stripped Skin Samples**; Eleanor Riches¹; Oliver O. Burt¹; Philippa J. Hart¹; Emmanuelle Claude¹; Malcolm R. Clench²; ¹Waters Corporation, Wilmslow, UK; ²Spectrometry Imaging, Biomolecular Sciences Research Centre, Sheffield Hallam University, Howard Street, Sheffield, UK
- TP 340 **Laden Latents: Revealing Human Handling of Psychoactive Plant Materials through Biomarker Fingerprint Imaging by MALDI-SpiralTOF High-Resolution Mass Spectrometry**; Cameron M. Longo¹; Rabi A. Musah¹; ¹University at Albany-SUNY, Albany, NY
- TP 341 **Mass Spectrometry Imaging of Neurotransmitters in Brain Tissue after Intake of Drugs of Abuse**; Ludovic Muller¹; Shelley N. Jackson¹; Amina S. Woods¹; ¹NIH/NIDA-IRP, Baltimore, MD
- TP 342 **Mass Spectrometry Imaging of Small Xenobiotics on *Danio rerio* : Influence of Molecular Profiles Modification as Potential Localization Asset**; Mathieu Tiquet¹; Marc Muller²; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, Liège, Belgium; ²GIGA-R : Biologie et génétique moléculaire, Liège, Belgium
- TP 343 **Optimizing Physical Properties of Formulations Using LAESI Mass Spectrometry**; Suresh Annangudi¹; Erin Gemperline²; Gary Gustafson²; Kyung Myung²; Jeffrey Gilbert²; Steve Wilson²; ¹Dow Agrosciences, Indianapolis, IN; ²Dow AgroSciences, Indianapolis, IN
- TP 344 **Localisation of Caffeoyl Quinates in Developing**



Beans of Robusta Coffee (*Coffea canephora*) ;

Gerhard Saalbach¹; Cathie Martin¹; James McCarthy²; Daniel Knevitt¹; ¹John Innes Centre, Norwich, Norfolk; ²Nestlé Research and Development Center Tours France, Tours, France

TP 345 **Visualization of Abscissic Acid and 12-Oxo-Phytodienoic Acid in Immature *Phaseolus vulgaris* L. Seeds Using Desorption Electrospray Ionization-Imaging Mass Spectrometry**; Hirofumi Enomoto¹; Takuya Senu¹; Futoshi Sato²; Eri Yumoto¹; Takao Yokota¹; Hisakazu Yamane¹; ¹Department of Biosciences, Faculty of Science and Engineering, Teikyo University, Utsunomiya, Japan; ²Waters Corporation, Shinagawa, Japan

TP 346 **Matrix-Assisted Laser Desorption/Ionization-Mass Spectrometry Imaging (MALDI-MSI) for Direct Visualization of Wheat Grain Metabolites**; Shabarath Nambiar¹; Robert Trengove¹; Sze How Bong¹; Joel Gummer¹; ¹Murdoch University, Murdoch, WA

TP 347 **GCIB-ToF-SIMS High Resolution Imaging of Cardiolipin Speciation in the Brain: Identification of Molecular Losses after Traumatic Injury**; L.J. Sparvero¹; Hua Tian²; Andrew A Amoscato¹; Anna Bloom²; Nicholas Winograd²; Valerian E Kagan¹; Hülya Bayır¹; ¹University of Pittsburgh, Pittsburgh, PA; ²Pennsylvania State University, State College, PA

TP 348 **Comparative Tissue Imaging for Disease Characterization Using DESI Coupled with Uniform Field Drift Tube Ion Mobility High Resolution Mass Spectrometry**; Ruwan T Kurulugama¹; Joseph H Kennedy²; Brian C Laughlin²; Justin M Wiseman²; George Stafford¹; John Fjeldsted¹; ¹Agilent Technologies Inc., Santa Clara, California; ²Prosolia Inc., Indianapolis, IN

TP 349 **Comparison of Laser Ablation Atmospheric Pressure Photoionization (LAAPPI) and Laser Ablation Electrospray Ionization (LAESI) in MS Imaging of Animal Tissue**; Juha-Pekka Hieta¹; Anu Vaikkinen¹; Heikki Räikkönen¹; Jaakko Kopra¹; Petteri Piepponen¹; Markus Haapala¹; Tiina J. Kauppila¹; ¹University of Helsinki, Helsinki, Finland

TP 350 **Spatial Mapping of Metabolites and Neurotransmitter in Rat Brain Sections Using DESI Ion Mobility Mass Spectrometry**; Anthony J. Midey¹; Hernando J. Olivos¹; Michael Batey²; Emmanuelle Claude²; Bindesh Shrestha³; ¹Waters Corporation, Beverly, MA; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; ³Waters Corp., Beverly, MA

INFORMATICS: MULTIOMICS INTEGRATION 351 - 369

TP 351 **Crosstalk: An Open and Flexible Network and Pathway Analysis Platform**; Sean Maxwell^{1,2}; Mark R. Chance^{1,2}; ¹Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; ²Department of Nutrition, Case Western Reserve University, Cleveland, OH

TP 352 **Multimomics Data Integration Using Anatomical Ontologies**; Magnus Palmblad¹; Leiden University Medical Center, Leiden, Netherlands

TP 353 **Proteogenomics Reveals a Complicated Feature of the Molecular Characteristics of Colorectal Cancer in AOM/DSS Mouse Model**; Qingfei Pan^{1,2}; Yingying Xie¹; Lylia Drici³; Yanxia Liu¹; Lei Sun¹; Honggang Huang³; Bo Wen²; Martin Røssel Larsen³; Xiaomin Lou¹; Yan Ren²; Lin Wu¹; Peter Roepstorff³; Siqi Liu^{1,2}; ¹Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; ²BGI-Shenzhen, Shenzhen, China; ³Protein Research Group, Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark

TP 354 **Proteogenomics of Adenosine-to-Inosine RNA Editing**

in Fruit Fly; Ksenia G Kuznetsova¹; Irina Y Ilina¹; Alexey L Chernobrovkin²; Svetlana E Novikova¹; Tatyana E Farafonova¹; Dmitry S Karpov³; Mark I Ivanov^{4,5}; Olga E Voronko¹; Victor G Zgodat¹; Roman A Zubarev²; Mikhail V Gorshkov^{4,5}; Sergei A Moshkovskii^{1,6}; ¹Institute of Biomedical Chemistry, Moscow, Russia; ²Karolinska Institute, Stockholm, Uppland; ³Engelhardt Institute of Molecular Biology, Moscow, Russia; ⁴Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia; ⁵Moscow institute of physics and technology, Dolgoprudnyj, Russia; ⁶Pirogov Russian National Research Medical University (RNRMU), Moscow, Russia

TP 355 **ProteomeGenerator: Integrative Proteomics and Transcriptomics for Non-Canonical Proteome Discovery**; Paolo Cifani¹; Avantika Dhabaria²; Akihito Yoshimi³; Omar I. Abdel-Wahab³; John T. Poirier^{1,4}; Alex Kentsis^{1,5}; ¹Molecular Pharmacology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY; ²New York University Langone Medical Center, New York, NY; ³Human Oncology & Pathogenesis Program, Memorial Sloan Kettering Cancer Center, New York, NY; ⁴Department of Medicine, Memorial Sloan Kettering Cancer Center, New York, NY; ⁵Department of Pediatrics, Weill Medical College of Cornell University and Memorial Sloan Kettering Cancer Center, New York, NY

TP 356 **Integrated Data Analysis Pipelines for Meta-Omics**; Sujun Li¹; Yuzhen Ye¹; Haixu Tang¹; ¹Indiana University, Bloomington, IN

TP 357 **Proteogenomics of Malignant Melanoma Cell Lines: Searching for Genetically Encoded Point Mutations in LC-MS/MS Data**; Anna Lobas¹; Alexey L Chernobrovkin²; Irina Ilina³; Dmitry S Karpov^{3,4}; Mikhail Pyatnitskiy³; Elizaveta M Solovyeva^{1,5}; Ksenia G Kuznetsova³; Mark I Ivanov^{1,5}; Roman Zubarev²; Mikhail V Gorshkov^{1,5}; Sergei A Moshkovskii³; ¹INEPCP RAS, Moscow, Russia; ²Karolinska Institute, Stockholm, Uppland; ³Institute of Biomedical Chemistry, Moscow, Russia; ⁴Engelhardt Institute of Molecular Biology, Moscow, Russia; ⁵Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia

TP 358 **A Linear Algebraic Approach to Combine Top Down and Bottom Up Data and Accurately Determine Protein Modform Distributions**; Philip Compton¹; Neil L Kelleher²; Jeremy Gunawardena³; ¹Northwestern University, Evanston, IL; ²Northwestern University, Evanston, IL; ³Harvard Medical School, Boston, MA

TP 359 **Automated Visualization of Metabolome, Proteome and Fluxome Data on Garuda – a Connectivity Platform for Biomedical Analytics**; Fumio Matsuda¹; Yohei Yamada²; Samik Ghosh³; Takeshi Hase³; Syohei Kinoshita¹; Shunsuke Nishino¹; Atsumi Tomita¹; Nikolaos Tsormas³; Atsuhiko Toyama²; Shigeki Kajihara²; Norio Mukai²; Yukiko Matsuoka³; Hiroshi Shimizu¹; Eiichiro Fukisaki¹; Hiroaki Kitano³; Junko Iida^{2,4}; ¹Osaka University, Suita, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³The Systems Biology Institute, Tokyo, Japan; ⁴Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan

TP 360 **Phenome Study on the Tissues of Esophageal Squamous Cell Carcinoma**; Guixue Hou¹; Shaohang Xu¹; Bo Wen¹; Xiaomin Lou²; Yan Ren¹; Jin Zi¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China; ²Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China

TP 361 **A Sparse Latent Regression Approach for Integrative Analysis of glycomic and Glycotranscriptomic Data**; Xuefu Wang¹; Sujun Li¹; Shiyue Zhou²; Yehia Mechref³; Haixu Tang³; ¹School of Informatics and Computing, Indiana University, Bloomington, IN - Indiana; ²Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; ³Indiana University, Bloomington, IN

TP 362 **Multi-Omic Informatics in the Cloud: Galaxy-P Takes a**



TUESDAY POSTERS

- Ride on Jetstream;** Tim Griffin¹; Matthew C. Chambers²; James E. Johnson^{1,3}; Thomas McGowan^{1,3}; Thomas Doak⁴; Jeremy Fischer⁴; Praveen Kumar¹; Pratik Jagtap¹; ¹University of Minnesota, Minneapolis, MN; ²Vanderbilt University, Nashville, TN; ³Minnesota Supercomputer Institute, Minneapolis, MN; ⁴Indiana University Bloomington, Bloomington, IN
- TP 363 **Blood Metabolomics and Transcriptomics Define Metabolic Axes of Human Immune Response to Herpes Zoster Vaccine;** Shuzhao Li¹; Dean P. Jones¹; Bali Pulendran¹; ¹Emory University, Atlanta, Georgia
- TP 364 **A Galaxy-Based, Multi-Staged, Two-Step Searching Pipeline for Improved Peptide Identification in Next Generation Proteomic Studies;** Praveen Kumar¹; James Johnson²; Thomas McGowan²; Candace R. Guerrero¹; Pratik Jagtap¹; Tim Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²Minnesota Supercomputer Institute, Minneapolis, MN
- TP 365 **Enhancing the Multi-omics Visualization Platform (MVP) Plug-in for Galaxy-based Applications;** Thomas McGowan^{1,2}; James Johnson^{1,2}; Pratik Jagtap¹; Praveen Kumar¹; Getiria Onsongo^{1,2}; Candace R. Guerrero¹; Tim Griffin^{1,3}; ¹University of Minnesota, Minneapolis, MN; ²Minnesota Supercomputer Institute, Minneapolis, MN; ³Center for Mass Spectrometry and Proteomics, St. Paul, MN
- TP 366 **Transcriptome and Proteome Co-Analysis of High-Fat Diet Induced Hepatic Changes;** Devin Lee Drew¹; Prasanna Rajagopal²; Michelle Puchowicz³; Daniela M. Schlatter³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Bengaluru, India; ³Case Western Reserve University School of Medicine, Cleveland, OH
- TP 367 **Proteogenomic Analysis of 31 Human Tissues;** Thomas Wieland¹; Dongxue Wang²; Björn Hallström³; Li-Hua Li²; Anna Asplund⁴; Mathias Wilhelm²; Frederik Ponten⁴; Mathias Uhlen³; Hannes Hahne¹; Bernhard Kuster⁵; ¹OmicScouts GmbH, Freising, Germany; ²Technical University of Munich, Freising, Germany; ³KTH Royal Institute of Technology, Stockholm, Sweden; ⁴Uppsala University, Uppsala, Sweden; ⁵Technical University Munich, Freising, Germany
- TP 368 **Examining Codon Usage as a Potential Marker of Extracellular Proteins in Microbes;** Alexander Cope^{1,2}; Michael Gilchrist¹; Robert L. Hettich²; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- TP 369 **MS-Helios: A Circos Wrapper to Visualize Multi-Omic Datasets;** Harald Marx¹; Joshua J. Coon¹; ¹University of Wisconsin-Madison, Madison, WI

INFORMATICS: PROTEIN ID AND QUANTIFICATION 370 - 378

- TP 370 **Multi-Q 2: Automated and Robust Isobaric Labeling Quantitation Analysis with Enhanced Graphical Visualization of Protein Ratio Clustering;** Ching-Tai Chen¹; Cheng-Wei Cheng¹; Wei-Jhe Hsu²; Hui-Yin Chang¹; Chu-Ling Ko³; T. Mamie Lih^{1,4}; Yi-Ju Chen⁴; Yu-Ju Chen⁴; Wen-Lian Hsu¹; Ting-Yi Sung¹; ¹Institute of Information Science, Academia Sinica, Taipei, Taiwan; ²Department of Electrical & Computer Engineering, Texas A&M University, College Station, TX; ³Department of Computer Science, National Chiao Tung University, Hsin Chu, Taiwan; ⁴Institute of Chemistry, Academia Sinica, Taipei City, Taiwan
- TP 371 **Automated Identification of Intact N-Linked Glycoproteins with Multiple Protein Search Engines;** Cheng-Wei Cheng^{1,2}; Wen-Lian Hsu³; Ting-Yi Sung³; ¹Bioinformatics Program, Taiwan International Graduate Program, Institute of Information Science, Academia Sinica, Taipei, Taiwan; ²Institute of Biomedical Informatics, National Yang-Ming University, Taipei, Taiwan; ³Institute of Information Science, Academia Sinica, Taipei, Taiwan

- TP 372 **An Enhanced High-Throughput Quantitation Pipeline to Facilitate Transformative Top-Down Proteomics in 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
- TP 373 **PyGrouper: A Gene-Level Inference and Quantification Algorithm for Bottom-Up Proteomics Data;** Alexander B. Saltzman¹; Mei Leng¹; Anna Malovannaya¹; ¹Baylor College of Medicine, Houston, TX
- TP 374 **Flexible Learning Infrastructure for Proteomics;** Christopher Wilkins¹; Justice DR Sefas¹; Aivett Bilbao Pena¹; Richard D. Smith¹; Ljiljana Pasa-Tolic¹; Samuel H. Payne¹; Jared B. Shaw¹; ¹Pacific Northwest National Laboratory, Richland, WA
- TP 375 **Building Peptide Spectra Library by Spectral Clustering Using Graphics Processing Units (GPUs);** Paul TO¹; Henry LAM¹; ¹Division of Biomedical Engineering and Department of Chemical and Biomolecular Engineering, Hong Kong University of Science and Technology, Hong Kong, Hong Kong
- TP 376 **Enhanced Ion Charging Effect of m-Nitro Benzyl Alcohol (m-NBA) on Protein and Peptides Characterization;** Dipankar Malakar¹; faraz rashid¹; Manoj Pillai¹; ¹ABSCIEX, Gurgaon, Haryana
- TP 377 **Automated Workflow for Host Cell Protein Monitoring by Mass Spectrometry: from Raw Data to Final Report;** Stefano Gotta¹; Genedata AG, Basel, Switzerland
- TP 378 **Application of Novel SILAC Analysis Software Proteolabels for Large-Scale Meta-Analysis of Phospho-Proteomes;** Andrew Collins^{1,2}; Antony McCabe^{1,2}; Augustine Amakiri¹; Ian Morns³; Robert Tonge⁴; Johannes P.C. Vissers⁴; Andrew R. Jones^{1,2}; ¹University of Liverpool, Liverpool, UK; ²Omic Analytics, Liverpool, UK; ³Waters Corporation, Newcastle upon Tyne, UK; ⁴Waters Corporation, Wilmslow, UK

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- TP 379 **Plasma Pyrolysis Mass Spectrometry for the Diagnosis of Leishmaniasis;** Amanda Kretsch¹; Guido F. Verbeck¹; ¹University of North Texas, Denton, TX
- TP 380 **Automatic Construction of t-SRM Methods from Unscheduled SRM Data Raw Files Using the Xcalibur Workbench;** Qingyu Song¹; Mike Senko¹; Derek Bailey¹; Balaram Barange¹; ¹Thermo Fisher Scientific, San Jose, CA
- TP 381 **Resonance Effects in a Linear Ion Trap Driven by Rectangular RF Waveforms and AC Signals Applied in Dipolar Mode;** Alexander Lekkas¹; Andreas Boatzidis¹; Dimitris Papanastasiou²; ¹Fasmatech Science & Technology, Athens, Greece; ²Fasmatech, Athens, Attiki
- TP 382 **A RF Transfer Interface Operable over an Extended Pressure Range for Gating High Mass Ions into an oTOF Mass Spectrometer;** Alexander Lekkas¹; Dimitris Papanastasiou²; Diamantis Kounadis¹; Emmanuel Raptakis¹; Gerard van der Laan³; Jan Commandeur³; ¹Fasmatech Science & Technology, Athens, Greece; ²Fasmatech, Athens, Attiki; ³MS VISION, Almere, Netherlands
- TP 383 **Energy resolved Mass Spectrometry (ER-MS) in UPLC Timescales Using an Orthogonal Acceleration Quadrupole ToF with Novel Fast Acquisition Architecture;** Martin Green¹; Jason wildgoose¹; Keith Richardson¹; Williams Jonathan¹; Martin Palmer¹; ¹Waters Corporation, Wilmslow, UK
- TP 384 **AcroMass MS Processor: a Flexible Data System in Ion Trap Mass Spectrometry for Intact Protein Analysis;** Szu-Wei Chou¹; Shih-Chieh Yang¹; Yao-Hsin Tseng¹; Yi-Kun Lee¹; Liang-Chun Fan¹; Chun-Yen Cheng¹; ¹AcroMass technologies, Inc., Taipei



- TP 385 **Design and Performance of a Second Generation Cyclic Ion Mobility-Enabled Q-ToF**; Kevin Giles¹; Jakub Ujma¹; Jason Wildgoose¹; Martin R. Green¹; Keith Richardson¹; David Langridge¹; Nick Tomczyk¹; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- TP 386 **A Flexible, Cheap, Easy to Construct, and Effective Heater for Small Diameter Polymeric Tubing**; Ryan T. Hilger¹; James R. Zimmerman¹; ¹Jonathan Amy Facility for Chemical Instrumentation, Purdue University, West Lafayette, Indiana
- TP 387 **Application of High Speed TSQ MS with a Prototype RF/DC Rod Driver to Pesticide Analysis**; Harald Oser¹; Hans Schweingruber¹; Michael Ugarov¹; QINGYU SONG²; Michael Konicek²; Claudia Martins¹; Neloni Wijeratne²; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific, San Jose, CA
- TP 388 **Realistic Ion Inputs and their Corresponding Instantaneous Current Demands**; Russell Jurek; ETP Ion Detect, Clyde, NSW
- TP 389 **New Innovations Implemented on the Q Exactive HF Mass Spectrometer**; Tabiwang N. Arrey¹; Eugen Damoc¹; Erik Couzijn¹; Jens Grote¹; Oliver Lange¹; Christian Thoenig¹; Kerstin Strupat¹; Catherina Crone¹; Anastassios Giannakopoulos¹; Thomas Moehring¹; Alexander Harder¹; ¹Thermo Fisher Scientific, Bremen, Germany
- TP 390 **Fully Automated Platform for Determination of Benzodiazepines in Serum**; Davide Vecchiotti¹; Claudio Ghilardi¹; Katharina Kern²; Stéphane Moreau³; Isabel Cabruja¹; ¹Shimadzu Italy, Milan, Italy; ²Recipe Chemicals + Instruments GmbH, Munich, Germany; ³Shimadzu Europe GmbH, Duisburg, Germany
- TP 391 **A High Performance OA-ToF Mass Spectrometer for Accurate Mass Measurement of Mobility Separated Ions**; Jason Wildgoose¹; Martin R. Green¹; Jakub Ujma¹; Kevin Giles¹; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- TP 392 **Run, MS, Run! Increasing System Robustness with Ion Control**; Brent Lefebvre¹; Yang Kang¹; Mauro Aiello¹; Bradley B Schneider¹; J.C. Yves Leblanc¹; ¹SCIEX, Concord, ON, ON
- TP 393 **Cluster Analysis of Small Organic Molecules by Means of a LTP-Twin-Trap Mass Spectrometer**; Björn Raupers¹; Claus Köster²; Tassilo Muskat¹; Jürgen Grottemeyer¹; ¹Inst. f. Phys. Chem der CAU zu Kiel, Kiel; ²Bruker Daltonics, Bremen, Germany
- TP 394 **ECD in an RF-Free Electromagnetostatic hv-ExD Cell on a High Resolution/High Throughput Q-Exactive Orbitrap Mass Spectrometer**; Kyle L. Fort¹; Albert J. R. Heck¹; Valery G. Voinov^{2,3}; Yury Vasil'ev^{2,3}; Joseph S. Beckman³; ¹Utrecht University, Utrecht; ²e-MSion, Corvallis, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR
- TP 395 **Ice Formation on Nanoparticles in a Molecular Flow Linear Quadrupole Ion Trap**; Denis Duft¹; Mario Nachbar^{1,2}; Thomas Dresch²; Thomas Leisner^{1,2}; ¹Institute for Meteorology and Climate Research – Atmospheric Aerosol Research, Karlsruhe Institute of Technology, Karlsruhe, Germany; ²Institute of Environmental Physics, Ruprecht-Karls-University Heidelberg, Heidelberg, Germany
- TP 396 **RF Trap with Paracell Geometry**; Ekaterina Zhdanova¹; Vasilij Eliferov¹; Igor Popov¹; Eugene (Evgeny) Nikolaev^{1,2,3}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²Skolkovo institute of science and technology, Skolkovo, Russia; ³Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia
- TP 397 **Implementation of 213 nm Ultra Violet Photo Dissociation (UVPD) on a Modified Orbitrap Fusion Lumos**; Christopher Mullen¹; Chad R Weisbrod²; Eugene Zhuk¹; Romain Huguet¹; Jae C Schwartz³; ¹Thermo Fisher Scientific, San Jose, CA; ²National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ³Thermo Fisher Scientific, San Jose, California
- TP 398 **A Comparative Study of Commercial Electrospray Ionization Sources for Qualitative and Quantitative Proteomic Studies**; Melissa R. Pergande¹; R.A.C. Rathnayake¹; Carol Haney-Ball²; Vadiraja Bhat³; Stephanie M. Cologna¹; ¹University of Illinois at Chicago, Chicago, IL; ²Agilent Technologies Inc., Santa Clara, California; ³Agilent Technologies, Inc., Wilmington, DE
- TP 399 **Improving MS Performance by Improving High Voltage Power Quality**; James Morrison¹; Gary Byfield²; ¹Brave-Blue, Manlius, NY; ²Advanced Energy Industries, Inc., Fort Collins, Colorado
- TP 400 **Determination of the Analytical Figures of Merit for the Qsight Triple Quadrupole**; Joshua Wilhide¹; Ian W Shaffer¹; William R LaCourse¹; ¹University of Maryland Baltimore County, Baltimore, MD
- TP 401 **Measurement of Effective Radial Geometry of Non-Hyperbolic Linear Ion Trap**; Chuan-Fan Ding; Fudan University, Shanghai, China

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- TP 402 **Exploring the Benefits and Unique Applications of Cold EI for LC-MS**; Svetlana Tszin¹; Tal Alon¹; Alexander B. Fialkov¹; Aviv Amirav¹; ¹Tel Aviv University, Tel Aviv, Israel
- TP 403 **CHARON PTR-ToF-MS: a New Method for Real-Time Measurement and Molecular-Level Characterization of Submicron Particulate Organic Matter**; Philipp Eichler¹; Markus Mueller^{1,2}; Andreas Klinger²; Armin Wisthaler^{1,3}; Alfons Jordan²; ¹Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria; ²IONICON Analytik GmbH., Innsbruck, Austria; ³Department of Chemistry, University of Oslo, Oslo, Norway
- TP 404 **Scint Transmission over the Internet Using Mass Spectrometry**; Fred Paul Mark Jjunju¹; Giannoukos Stamatiou¹; DANIEL McGuiness¹; Alan Marshall¹; Valerio Selis¹; Jeremy Smith¹; Simon Maher¹; Stephen Taylor¹; ¹Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK
- TP 405 **Pyrolysis-Vacuum Assisted Plasma Ionization Ion Mobility-Mass Spectrometry for Insoluble Polymer Analysis**; Stephen Zambrozky¹; Matthew C Bernier²; James Bradshaw³; Facundo M Fernandez⁴; ¹Georgia Institute of Technology, Atlanta, Georgia; ²Georgia Institute of Technology, Atlanta, GA; ³Y-12 National Security Complex, Oak Ridge, Tennessee; ⁴Georgia Institute of Technology, Atlanta, GA
- TP 406 **Radio Frequency Powered Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Ionization Source for Atomic Mass Spectrometry**; Tyler Williams¹; Kenneth Marcus¹; ¹Clemson University, Clemson, SC
- TP 407 **Desorption Ionization Using Through Hole Alumina Membrane (DIUTHAME)**; Yasuhide Naito¹; Takayuki Ohmura²; Masahiro Kotani²; ¹GPI, Hamamatsu, Japan; ²Hamamatsu Photonics K.K., Iwata, Japan
- TP 408 **Development of a New Atmospheric Pressure Plasmaspray Ionization and Its Comparison with Electrospray Ionization**; Ping Cheng; School of Environmental and Chemical Engineering, Shanghai University, Shanghai, Shanghai
- TP 409 **Numerical Simulation of Ion Transport in a Nano-Electrospray Ion Source**; Wei Wang^{1,2}; Steve Bajic¹; Benzi John²; David Emerson²; ¹Waters Corporation, Wilmslow, UK; ²STFC Daresbury Laboratory, Warrington, UK
- TP 410 **Rapid Analysis of Liquid Food Products and Beverages Using Ultrasonic Rapid Evaporative Ionisation Mass Spectrometry**; Daniel Simon¹; Tamas Karancsi¹; Steven Derek Pringle²; Zoltan Takats³; ¹Waters Research Center,



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- Budapest; ²Waters Wilmslow UK, Wilmslow, Cheshire; ³Imperial College, London, UK
- TP 411 **Improving the Sensitivity of ESI-MS by Efficient Ion Transmission and Desolvation;** Chinthaka A. Seneviratne¹; Milad Nazari¹; Elizabeth S. Hecht¹; Jung Lee²; Peter Kottke²; Matthew Torres³; Andrei G. Fedorov²; David C. Muddiman¹; ¹W.M. Keck FTMS Laboratory for Human Health Research, Dept. of Chemistry, North Carolina State University, Raleigh, NC; ²The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA; ³School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA
- TP 412 **Charge Reduction and Novel Fragmentation of mAbs with an ESI/Impactor API Source;** Steve Bajic¹; Jeff Brown¹; ¹Waters Corporation, Wilmslow, UK
- TP 413 **Spray Mechanism in Contained-electrospray Ionization Investigated Using On-line Protein Modification;** Colbert Miller¹; Abraham K. Badu-Tawiah¹; ¹Ohio State University, Columbus, OH
- TP 414 **Analysis in Real Time Using Mass Spectrometry Coupled with Plasmas;** Joel Lemaire¹; Michel Heninger¹; Essyllt Louarn¹; Helene Mestdagh¹; Gérard Bauville²; Nicole Blin Simiand²; Blandine Bournonville²; Michel Fleury²; Kristaq Gazeli²; Stephane Pasquiers²; Sebastien Thomas^{1,2}; Joao Santos Sousa²; Elsa Bauchard³; Julien Leprovost³; ¹LCP, UMR8000, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France; ²LPGP, UMR8578, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France, Orsay, France; ³AlyXan, Juvisy sur Orge, France
- TP 415 **Secondary Ion Mass Spectrometry with Individual Projectiles: A Complete Mass Spectrum from a Single Impact?**; Michael J. Eller¹; Anita Vinjamuri¹; Gabriel D. Shuffield¹; Bryan Tomlin¹; Emile A. Schweikert¹; ¹Texas A&M University, College Station, TX
- TP 416 **Improving Spray Stability in Negative Mode Nano-ESI with a Novel Coaxial Sheath Spray Device;** Samuel Wein¹; Benjamin A. Garcia²; ¹University of Pennsylvania, Philadelphia, Pa; ²University of Pennsylvania, Philadelphia, PA
- TP 417 **DRy Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement via Inertial Sorting;** Jung Lee¹; Peter A. Kottke²; Elizabeth S. Hecht³; Chinthaka A. Seneviratne³; David C. Muddiman³; Alex P. Jonke¹; Matthew P. Torres²; Andrei G. Fedorov²; ¹Georgia Institute of Technology, Atlanta, GA; ²Georgia Institute of Technology, Atlanta, GA; ³North Carolina State University, Raleigh, NC
- TP 418 **Characterization of Labile Highly Sulfated Cyclodextrins (HSCD) by Cold-Spray Ionization (CSI) Mass Spectrometry;** Daniel Ortiz¹; Samuel Jones¹; Francesco Stellacci¹; Laure Menin¹; ¹École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- TP 419 **Ultra High Resolution Atmospheric Pressure Chemical Ionization Evolved Gas Analysis - Gas Chromatography and Thermal Analysis Applied for Petroleum Analysis;** Christopher Paul Rüger¹; Theo Schwemer^{1,2}; Anika Neumann¹; Martin Sklorz¹; Uwe Kaefer^{3,4}; Thomas Groeger³; Ralf Zimmermann^{1,2,5}; ¹Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ²HICE – Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu, Neuherberg, Germany; ³Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, München, Germany; ⁴ASG Analytik Service-Gesellschaft mbH, Neusäss, Germany; ⁵Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany
- TP 420 **Development and Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis;** Felipe Lopez-Hilfiker^{1,2}; Sonja Klee¹; Veronika Pospisilova²; Manuel Hutterli¹; Jay Slowik²; Andre Prevot²; Urs Baltensperger²; ¹TOFWERK, Thun, Switzerland; ²Paul Scherrer Institute (PSI), Villigen, Switzerland
- TP 421 **Matrix-Free Laser Desorption/Ionization Using Microstructured Anti-Reflection Metal Surfaces;** Jing Yang¹; Xiaoxiao Ma¹; Zishuai Li¹; Jia Jia²; Peixun Fan³; Minlin Zhong³; Zheng Ouyang^{1,4}; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ²Department of Chemistry, Tsinghua University, Beijing, China; ³School of Materials Science and Engineering, Tsinghua University, Beijing, China; ⁴Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN
- TP 422 **H2-Plasma for the Generation of Protonation Reagents with a Standard APPI Power Supply;** Hendrik Kersten¹; Tobias Kutsch¹; Kai Kroll¹; Kirsten Haberer¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal
- TP 423 **A New Atmospheric Pressure Ionization Source Using a High Voltage Target Compared to Electrospray Ionization;** Arnaud Lubin¹; Steve Bajic²; Deirdre Cabooter³; Patrick Augustijns³; Filip Cuyckens¹; ¹Janssen R&D, Beerse, Belgium; ²Waters Corporation, Wilmslow, UK; ³Department of Pharmaceutical and Pharmacological Sciences, Leuven, Belgium
- TP 424 **Evaluation of a Kinetically Controlled Chemical Ionization Setup;** Kai Kroll¹; Duygu Erdogdu¹; Tobias Kutsch¹; Hendrik Kersten¹; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW
- TP 425 **Improvement of μpCl for Proton Transfer Reactions: a Chambered Ion Source Design for Suppression of Water-Cluster;** Nele Hartmann¹; David Mueller¹; Robin Hillen¹; Yessica Brachthäuser¹; Klaus J. Brockmann¹; Hendrik Kersten¹; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW
- TP 426 **nESI-MS Measurement of Protein Melting Temperature Using θ Tip Electroosmosis Induced Joule Heating Effect;** Feifei Zhao¹; Jiexun Bu²; Sarah M Matt²; Owen G. Rehrauer³; Dor Ben-Amotz²; Scott A McLuckey²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN; ³Vertex Pharmaceuticals, Boston, MA
- TP 427 **Adjustable In-Source Fragmentation of Metabolites and Lipids in Laser Desorption Ionization from Silicon Nanopost Arrays;** Andrew Korte¹; Akos Vertes²; ¹George Washington University, Washington, DC; ²George Washington University, Washington, DC
- TP 428 **Atmospheric Pressure Temperature Ramped Thermal Desorption/Ionization – Atomic Force Microscope/Mass Spectrometry System for Spatially Resolved Surface Analysis;** Vilmos Kertesz¹; William D. Hoffmann¹; Gary J. Van Berkel¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- TP 429 **Pulsed Valve Inlet Ionization;** Bijay Banstola¹; Md Amir Hossen¹; Fabrizio Donnarumma¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 430 **Development of an Adaptable, High Sensitivity, Automation for Inlet Ionization;** Milan Pophristic¹; Sean Rayna²; Kevin Rackers²; Anil Meher^{1,3}; I-Chung Lu³; Ana Djuric⁴; Sarah Trimpin^{1,3}; Charles McEwen¹; ¹MSTM, LLC., Newark, DE; ²Automation Techniques, Inc, Greensboro, NC; ³Department of Chemistry, Wayne State University, Detroit, MI; ⁴Engineering Technology, Wayne State University, Detroit, MI
- TP 431 **Electrode-Less Secondary Electrospray Ionization (SESI) for Breath Analysis: Improving the Limits of Detection for Low Volatility Species;** Guillermo Vidal-de-Miguel¹; Miriam Macia¹; Pablo Martinez-Lozano Sinues²;



¹Fossil Ion Technology, Madrid, Spain; ²ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland

- TP 432 **Comparison of Electrospray and Impactor Ionization for Pharmaceutical Compounds;** Kerri M Smith¹; Yun Alelyunas¹; Giorgis Isaac¹; Joe LaPointe²; Nigel Ewing¹; Mark D Wrona¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA
- TP 433 **Spark Discharge Ablation and Ionization of Metalliferous Aerosol Particles;** Thorsten Benter¹; Joshua Rieger¹; Steffen Bräkling¹; Hendrik Kersten¹; ¹University of Wuppertal, Wuppertal, Germany
- TP 434 **100% Input Efficient ESI UPLC MS Sample Introduction and MALDI, SIMS, LDI Sample Placement via an Inductive Approach. Universal ?;** Drew Sauter¹; Andrew D. Sauter¹; Patrick A. Limbach²; Robert Ross²; Manasses Jora²; ¹Nanoliter, LLC, Henderson , NV; ²University of Cincinnati, Cincinnati, OH

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- TP 435 **Analysis of Perfluorinated Compounds in Water Using Automated Solid Phase Extraction;** Rudolf Addink¹; Rashid Juma¹; ¹Toxic Report, Watertown, MA
- TP 436 **Determination of Artificial Sweeteners in Water Samples by Liquid-Phase Microextraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry;** Yu-Hsin Lin¹; Chung-Yu Chen¹; Maw-Rong Lee¹; ¹National Chung-Hsing University, Taichung, Taichung
- TP 437 **Effective Simultaneous Determination of Five Estrogens in Aqueous Samples Using DLLME and LC-MS/MS;** Seung-Woon Myung¹; Yeon-Joo Moon¹; Jun Seok Kim²; ¹Kyonggi University, Suwon-si, South Korea; ²Korea Polytechnics, Seongnam-si, South Korea
- TP 438 **HPLC/MS/MS Quantitation of Dopamine in Rat Plasma Using AAO Extraction and Derivatization;** Rachel Sun¹; Tim Shoaf¹; Robert Clegg¹; Adrian Bott¹; ¹BASi, West Lafayette, IN
- TP 439 **iST: a Reproducible Sample Preparation Method for In-Depth Proteome Discovery and Interaction Proteomics;** Fabian Hosp¹; Garwin Pichler¹; Nils A. Kulak¹; Matthias Mann²; ¹PreOmics, Planegg/Martinsried, Bavaria; ²Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 440 **Measurement of Pesticides in Apple Juice Using LC-MS/MS with Fast and Modified QuEChERS Extraction Method Using Volatile Buffers;** Avinash Dalmia¹; Reza Javahery²; Lisa Cousins²; Scott Lapaglia³; Wilhad Reuter³; Frenny Kaushal⁴; David welkie³; ¹PerkinElmer, Shelton, CT; ²PerkinElmer, Woodbridge, ON; ³PerkinElmer, Shelton , CT; ⁴PerkinElmer, Bolton, ON
- TP 441 **A Robust Protocol for Detergent-Free Cell Lysis, Protein Enrichment and Modification with a High Tolerance for Harsh Conditions;** Yannik Lewin; Department of Pharmaceutical Chemistry, Goethe University, Max-von-Laue-Straße 9, D-60438, Frankfurt am Main, Germany
- TP 442 **Fully Automated Online Sample Preparation and LC-MS/MS Analysis of Drugs of Abuse in Oral Fluids;** Joshua E. Emory¹; Michael Roberts¹; Manoj Tyagi²; Brian Feild¹; ¹Shimadzu Scientific Instruments, Columbia, MD; ²Captiva Lab, LLC, Charlotte, North Carolina
- TP 443 **Assessment of Solvent Polarity upon Drugs of Abuse in Oral Fluids Using Supported Liquid Extraction (SLE) prior to LC/MS Analysis;** Dan Menasco¹; Jillian Neifeld¹; Bruce Kempf¹; Stephanie J Marin¹; Elena Gairloch¹; Helen Lodder²; Alan Edgington²; Adam Senior²; Lee Williams²; Paul Roberts²; Claire Desbrow²; Steve Jordan²; ¹Biotage, Charlotte, NC; ²Biotage GB Limited, Cardiff
- TP 444 **Comparison of Novel β -Glucuronidases for Process Improvement in Urine Toxicology Workflows;** Phillip R. Gibbs¹; Hannah M. Milano¹; Matthew D. Kibbons¹; ¹Clinical Lab Consulting of Indiana, LLC, Indianapolis, IN - Indiana
- TP 445 **Simultaneous Extraction of Catecholamine and Metanephrines from Urine Prior to UHPLC-MS/MS Analysis;** Alan Edgington¹; Adam Senior¹; Lee Williams¹; Rhys Jones¹; Helen Lodder¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹Biotage GB Limited, Cardiff
- TP 446 **Thermostable Trypsin/Lys-C Facilitates High-Throughput, Automated Proteomics Sample Preparation for Complex Samples;** Carrie Romer¹; Danielle B. Gutierrez¹; Jamie L. Allen¹; Yuan-wei Nei¹; Melissa A. Farrow²; Nikesh Dahal²; Jocelyn Simpson²; Salisha Hill¹; Kristie L. Rose¹; Jeremy L. Norris¹; Michael Rosenblatt³; Eric P. Skaar²; D. Borden Lacy²; Richard M. Caprioli¹; ¹MSRC Vanderbilt University, Nashville, TN; ²Vanderbilt University Medical Center, Nashville, TN; ³Promega Corporation, Madison, WI
- TP 447 **Screening and Quantitation of over 200 Pesticides/Antibiotics in Honey Using the eXtremeFV for Sample Prep and On-Line Extraction UHPLC-MS/MS Analysis;** Sam Ellis; Thomson Instrument Company, Oceanside, CA
- TP 448 **Electromagnetic Mixer for Highly Efficient, Automated Sample Preparation;** Chang Liu¹; Don W Arnold²; Thomas R. Covey¹; ¹SCIEX, Concord, ON; ²SCIEX, Redwood City, CA
- TP 449 **Method Optimization for the Low Level Detection of Vitamin B7 from Human Serum Using UPLC-MS/MS Analysis;** Lee Williams¹; Helen Lodder¹; Rhys Jones¹; Alan Edgington¹; Adam Senior¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹Biotage GB Limited, Cardiff
- TP 450 **Therapeutic Drug Monitoring of Antiepileptic Drugs in Serum: a Fully Automated Approach;** Davide Vecchiatti¹; Claudio Ghilardi²; Stéphane Moreau³; Stephan Schröder⁴; Katharina Kern⁵; Isabel Cabruja²; ¹Shimadzu, Milan, Lombardy; ²Shimadzu Italy, Milan, Italy; ³Shimadzu Europe GmbH, Duisburg, Germany; ⁴Shimadzu Deutschland GmbH, Duisburg, Germany; ⁵Recipe Chemicals + Instruments GmbH, Munich, Germany
- TP 451 **Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis;** Limian Zhao¹; Derick Lucas²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Inc., Wilmington, DE
- TP 452 **Online Extraction of Antihypertensive Drugs from Human Serum Samples by LC-MS/MS Analysis;** Carolina Tosin Bueno¹; Henrique Dipe de Faria²; Eduardo Costa Figueiredo²; Jose Eduardo Krieger¹; Eduardo Moacyr Krieger¹; Alexandre Costa Pereira¹; Paulo Caleb Junior Lima Santos¹; ¹Laboratory of Genetics and Molecular Cardiology, Heart Institute (InCor), University of Sao Paulo, Medical School, Sao Paulo, Brazil; ²Laboratory of Toxicant and Drug Analysis, University of Alfenas - Unifal-MG, Alfenas, Brazil
- TP 453 **Development of a Simple and Sensitive Derivatization Method for LC/MS/MS Analysis of Epinephrine in high Salt Contained Buffer Solutions;** Bih-Hsiung Hsu¹; Patrick Lin¹; ¹PHARMout Lab, Sunnyvale, CA
- TP 454 **LC/MS/MS Bioanalytical Protocol for Determining the Degree of Non-Specific Binding in Multi-Well Plates;** Liyun Zhang¹; Jack Henion¹; ¹Q2 Solutions, Ithaca, NY
- TP 455 **LC-MS/MS Assay Miniaturization in Support of ABS Microsampling Pharmacokinetics Studies;** Elizabeth A. Mahan¹; Ken Anderson²; Jacqueline Kenny²; Rena Zhang²; ¹Merck & Co., West Point, PA; ²Merck & Co., West Point, PA
- TP 456 **Comparison of Manual and Automated Sample Preparation Techniques for Lipidomics;** Linda Ahonen¹; Peter Rossing¹; ¹Steno Diabetes Center Copenhagen, Gentofte, Denmark



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- TP 457 **Sample Preparation Strategies for Urine Panels with 50 of More Drugs and Metabolites Analyzed by LC-MS/MS;** Stephanie J. Marin¹; Dan Menasco¹; Jillian Neifeld¹; Elena Gariloch¹; ¹*Biotage, Charlotte, NC*
- TP 458 **Quantitative Analysis of THC and related cannabinoids in Multiple Matrices Using Simplified Solid Phase Extraction with UPLC/MS/MS;** XIN ZHANG¹; Jonathan Danaceau²; Erin Chambers²; Kim Haynes²; ¹*Waters Corp, Milford, MA*; ²*Waters Corporation, Milford, MA*
- TP 459 **Improved LC/MS/MS Analysis of Vitamin D Metabolites in Biological Samples Using Enhanced Matrix Removal Sample Preparation** ; Derick Lucas¹; Limian Zhao²; ¹*Agilent Technologies, Wilmington, DE*; ²*Agilent Technologies, Inc., Wilmington, DE*
- TP 460 **Development of a LC-MS/MS Method for Quantitative Measurement of Drugs in Microscale 3D Bioprinted Human Liver Samples;** Emily Adarayan¹; Elizabeth A. Mahan¹; Guangping Bi¹; Gary Adamson¹; Rena Zhang¹; Andreas Baudy¹; ¹*Merck Reseach Labs, West Point, PA*
- TP 461 **Organic Flush Solutions to Remove Sample Matrix Interferences in LC-MS Systems** ; Haibo Wang¹; Stephen C Roemer²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Fair Lawn, NJ - New Jersey*
- TP 462 **Optimized SPE-LC/MS/MS Assay to Support Measurement Released Drug in Nanoparticle Formulation** ; Wei Song¹; Brian Rago¹; Yizhong Zhang¹; Eyoung Shin¹; Young-Ho Song¹; Aarif Ahsan¹; Ravi Visswanathan¹; Mauricio Leal¹; Chris Holliman¹; ¹*Pfizer, Groton, CT*
- TP 463 **Drugs of Abuse in Oral Fluids: Automated SPE Extraction and LC/MS/MS Analysis Using a Robotic Autosampler;** Fred Foster¹; John R. Stuff¹; Edward A. Pfannkoch¹; Mark Hayward²; ¹*Gerstel, Inc., Linthicum , MD*; ²*ITSP Solutions, Hartwell, GA 30643*
- TP 464 **Method Development Strategies Using Polymer-Based SPE for the Analysis of Peptides Prior to UPLC-MS/MS Analysis;** Helen Lodder¹; Lee Williams¹; Rhys Jones¹; Adam Senior¹; Alan Edgington¹; Geoff Davies¹; Steve Jordan¹; Claire Desbrow¹; Paul Roberts¹; ¹*Biotage GB Limited, Cardiff, UK*
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- TP 465 **Facile Analysis of Sterols by Thiol-Based Photochemical Tagging and Electrospray Ionization – Mass Spectrometry;** Sarju Adhikari¹; Yu Xia¹; ¹*Purdue University, West Lafayette, Indiana*
- TP 466 **Study on Triacylglycerides in Edible Vegetable Oils by Ultra-High Performance Liquid Chromatography Tandem Quadrupole-Time Of Flight Mass Spectrometry;** Jianzhong Li¹; Yao Xiao²; Xin Ma²; Qilei Guo²; Tao Bo²; ¹*Agilent Technologies(China), Beijing, Beijing*; ²*Agilent Technologies (China), Beijing, China*
- TP 467 **Comprehensive Analysis of N-Acylethanolamine and Monoacylglycerol Species by Shotgun Lipidomics;** Kazuo Kanaya¹; Miao Wang¹; Xianlin Han¹; ¹*Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*
- TP 468 **Effects of Heparin Versus EDTA Anti-Coagulant on Plasma Samples Analyzed Using the LipidizerTM Platform;** Richard J. Robinson¹; Philip M. Charpia¹; Uyenthao T. Nguyen¹; Anne M. Evans¹; Luke A.D. Miller¹; ¹*Metabolon, Inc., Durham, NC*
- TP 469 **Evaluation of Hepatic Lipids from Rabbits under Conditions Stimulating Non-Alcoholic Fatty Liver Disease Using Nanoflow UPLC-ESI-MS/MS;** Seul Kee Byeon¹; Myeong Hee Moon¹; ¹*Yonsei University, Seoul, South Korea*
- TP 470 **Shotgun Lipidomics Reveals Decreases in Myelin Lipid Content in the Central and Peripheral Nervous Systems of db/db Mice;** Chunyan Wang¹; Palavicini Pablo Juan¹; Linyuan Chen¹; Jianing Wang¹; Xianlin Han¹; ¹*Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*
- TP 471 **Probing the Electrostatic Interactions between Cationic Antimicrobial Peptides and Kdo2-Lipid A via Ultraviolet Photodissociation Mass Spectrometry;** Christopher M. Crittenden¹; Lindsay J Morrison¹; Lucas D Akin¹; Bryan W Davies^{2,3}; Jennifer S Brodbelt¹; ¹*Department of Chemistry, University of Texas at Austin, Austin, TX*; ²*Department of Molecular Biosciences, University of Texas at Austin, Austin, TX*; ³*Institute of Cellular and Molecular Biology, University of Texas at Austin, Austin, TX*
- TP 472 **HCD-Analysis of Human Blood Plasma Lipid Classes via Combinatorial Free Fatty-Acid and Solid Phase Extraction of Phospho-, Glycero-, and Sphingolipids;** Tobias M Maile¹; Eugene Melamud¹; Bryson Bennett¹; ¹*Calico LLC, South San Francisco, CA*
- TP 473 **Lipid Parameters Associated with Obesity Identified Using a High-Throughput Shotgun Lipidomics Technology;** Christian Klose¹; Michal A. Surma¹; Ronny Herzog¹; Mathias Gerl¹; Elena Sokol²; David Peake³; Céline Fernandez⁴; Olle Melander^{4,5}; Kai Simons¹; ¹*Lipotype GmbH, Dresden, Saxony*; ²*Thermo Fisher Scientific, Hemel Hempstead, UK*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Department of Clinical Sciences, Lund University, Malmö, Sweden*; ⁵*Department of Internal Medicine, Malmö, Sweden*
- TP 474 **Recent Improvements in TrEnDi: Lipid Scope and Signal Consolidation;** Carlos R. Canez¹; Gilian T. Thomas¹; Samuel W.J. Shields¹; Karl V. Wasslen¹; Peter J. Pallister¹; Jeffrey M. Manthorpe¹; Jeffrey C. Smith¹; ¹*Carleton University, Ottawa, ON*
- TP 475 **Size Fractionation Coupled to Lipid and Protein Measurements to Quantify Lipoprotein Particle Number and Composition in Normal and Dyslipidemic Subjects;** Michael Gardner¹; Zsuzsanna Kuklenyik¹; David M Schieltz¹; Bryan A Parks¹; Jon Rees¹; Lisa McWilliams¹; Christopher Toth¹; Jeffrey Jones¹; Michael Andrews¹; Antony Lehtikoski¹; John Barr¹; ¹*Centers for Disease Control and Prevention, Atlanta, GA*
- TP 476 **Identification and Quantification of Lecithin Phospholipid in Freeze Dried and Drum Dried Fruit and Vegetable by LC-MS and HPLC-ELSD;** Xiaoyan Xia¹; Boris V. Nemzer^{2,3}; ¹*FutureCeuticals Inc., Mokence, IL*; ²*FutureCeuticals Inc., Mokence, IL*; ³*Department of Food Science and Human Nutrition, University Illinois at Urbana Champaign, Urbana, IL*
- TP 477 **Quantitation of Phospholipids Based on Isotope-Labeled Methylation Using nUPLC-ESI-MS/MS;** Jong Cheol Lee¹; Seul Kee Byeon¹; Myeong Hee Moon¹; ¹*Yonsei University, Seoul, South Korea*
- TP 478 **Fragmentation Behavior of Neuronal Lipids by HCD-MS/MS;** Tommy Hofmann¹; Carla Schmidt¹; ¹*Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany*
- TP 479 **Synaptamide Biosynthesis Monitored by Stable Isotope Labeling and High Resolution Mass Spectrometry;** Karl Kevala¹; Michel Lagarde²; Arthur Spector¹; Hee-Yong Kim¹; ¹*National Institutes of Health, NIAAA, Rockville, MD*; ²*Universite de Lyon, INSA, Villeurbanne, France*
- TP 480 **Automated Lipid Profiling of a Plasma Sample Using Ultra-High Resolution Qq-Time-Of-Flight Impact II™ Mass Spectrometer with SimLipid Software;** Ningombam Sanjib Meitei¹; Himani Gupta¹; Arun Apte²; Aiko Barsch³; Anjali Alving⁴; Juan J Aristizabal Henao⁵; Ken D Stark⁵; ¹*PREMIER Biosoft, Indore, India*; ²*PREMIER Biosoft, Palo Alto, CA*; ³*Bruker Daltonik GmbH, Bremen, Germany*; ⁴*Bruker Daltonik, Billerica, MA*; ⁵*University of Waterloo, Waterloo, Ontario*



- TP 481 **Lipidomic Analysis of Urinary Exosomes According to their Sizes by Flow Field-Flow Fractionation and nUPLC-ESI-MS/MS;** Joon Seon Yang¹; Myeong Hee Moon¹; ¹Yonsei University, Seoul, South Korea
- TP 482 **The Role of Decreased Mitochondria Phospholipid and Impaired Electron Transport Chain for Brain Damage in Cardiac Arrest**; Jonathan Tam¹; Angela Hong²; Tai Yin³; Junhwan Kim³; ¹Hofstra Northwell School of Medicine, Hempstead, NY; ²Villanova University, Villanova, PA; ³Feinstein Institute for Medical Research, Manhasset, NY
- TP 483 **Investigating the Pathways of Lipid Biosynthesis in *C. reinhardtii* under Nitrogen Starvation Conditions Using Isotope Labeling and LC-MS;** Carter Lantz¹; Matthew Brantley¹; James Chang¹; Jeremy Sieker¹; Sung-Joon Kim¹; Touradj Solouki¹; ¹Baylor University, Waco, Texas
- TP 484 **Authentication of Two Different Types of Fish Oils by Qualitative Lipid Profiling Using Semi-Targeted Approach on QTRAP Platforms;** Niladri Sekhar Chatterjee¹; Akanksha Singh²; Vishnu KV¹; Ajeeshkumar K K¹; Anandan R¹; Ashok Kumar¹; Suseela Mathew¹; Manoj Pillai²; ¹ICAR-Central Institute of Fisheries Technology, Cochin, India; ²SCIEX, 121, Udyog Vihar, Phase IV, Gurugram, India
- TP 485 **Identification of Ligands for YF1*7.1, a Novel MHC Class I-Like Molecule;** Gabriel Gugiu^{1,2}; Ronald Goto³; Marcia Miller³; ¹City of Hope, Molecular immunology - BRI, Duarte, CA; ²City of Hope, Shared Resources - BRI, Duarte, CA; ³City of Hope, Molecular & Cellular Biology - BRI, Duarte, CA
- TP 486 **Enhanced Coverage of Lipid Analysis and Imaging by MALDI-MS via a Strategy with an Optimized Mixture of Matrices;** Jianing Wang¹; Chunyan Wang¹; Xianlin Han¹; ¹Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL
- TP 487 **Comprehensive Global Lipidomics Profiling on LC-MS/MS Timeframe with Quadrupole Orbitrap Mass Spectrometer Detection;** Josef Ruzicka¹; David A. Peake²; ¹Thermo Fisher Scientific, Somerset, NJ; ²ThermoFisher, San Jose, CA
- TP 488 **Next Generation Lipid Profiling of Human Red Blood cells Unmasks Hidden Diversity;** Amani M Batarseh¹; Sarah K Abbott¹; Ayedh Alqarni¹; Stephen J Blanksby²; Todd W Mitchell¹; ¹University of Wollongong, Wollongong, NSW; ²Queensland University of Technology, Brisbane, Australia
- TP 489 **Lipidomic Responses of Stem Cells to Microfabricated Structures Using MALDI-MS;** Martin R. L. Paine¹; Nick R. M. Beijer²; Jan De Boer²; Ron M. A. Heeren¹; Shane R. Ellis¹; ¹M4I Institute - Maastricht University, Maastricht, Netherlands; ²MERLN Institute, Maastricht, Netherlands
- TP 490 ***in situ* and Plasma Phospholipidome Studies of Rats Following Ischemic Stroke;** Hay-Yan J. Wang¹; Erh-Hsuan Hsiang¹; Zhi-Fu Zheng²; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Hyper Quantum Technologies, Kaohsiung, Taiwan
- TP 494 **Enhancing Ion Abundances of Carbohydrates by Controlling Sample Crystalline Structures in MALDI Mass Spectrometry;** Yu-Meng Ou^{1,2}; Hsun Lee¹; Yin-Hung Lai¹; Huan-Tsung Chang²; Yi-Sheng Wang¹; ¹Genomics Research Center Academia Sinica, Taipei; ²Department of Chemistry, National Taiwan University, Taipei, Taiwan
- TP 495 **Non-Commercial MALDI Matrices for the Analysis of Acidic Peptides;** Xinyao Jing¹; Kyle Edwards¹; John B. Vincent¹; Angelo James¹; Yuping Bao¹; Carolyn J Cassidy¹; ¹The University of Alabama, Tuscaloosa, AL
- TP 496 **Improved Quantitative Analysis in MALDI-MS Using Freeze Vacuum Drying;** Dongwon Shin¹; Jihyun Paek¹; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, Daejeon
- TP 497 **Coffee Ring Effect Enhancement of Biomolecule Signals by MALDI;** Laura J Castellanos-Garcia¹; Alyssa L. M Marsico¹; Bradley Duncan¹; Ryan F. Landis¹; Gulen Yesilbag Tonga¹; Vincent M Rotello¹; Richard W Vachet¹; ¹University of Massachusetts-Amherst, Amherst, MA
- TP 498 **Effect of Additive Cation on the Analysis of Sucrose Using MALDI-MS;** Jihyun Paek¹; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, Daejeon
- TP 499 **New Fixed-Charge Derivatization Agents for Analysis of Carbonyl Compounds by MALDI, SALDI and ESI Mass Spectrometry;** Larisa Kulikova¹; Valentina Ilyushenkova¹; ²Dmitrii Zhilyaev^{1,2}; Roman Borisov^{1,3}; ¹RUDN University, Moscow, Russia; ²Topchiev Institute of Petrochemical synthesis, Moscow; ³Topchiev Institute of Petrochemical synthesis, Moscow
- TP 500 **Combined Solid and Liquid Matrix High Vacuum Sublimation and Evaporation Coating for MALDI Imaging;** Fan Cao¹; Fabrizio Donnarumma¹; Md Amir Hossen¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 501 **Covalent Linkage of Matrix for Enhanced MALDI-MS;** Jason Williams; NIEHS, RTP, NC
- TP 502 **Development of a Novel Sample Preparation Approach for Bottom-Up Shotgun Proteomics;** Simona Salivo¹; Tom K. Abban¹; Emanuele Barborini²; Matthew E. Openshaw¹; ¹Shimadzu, Manchester, UK; ²Tethis SpA, Milan, Italy
- TP 503 **Direct On-Plate Desalting and Enrichment for Improved Low Molecular Weight Marker Detection;** Mohamed Nazim Boutaghou¹; Sharath Hosali²; Jason Sakamoto²; Brian Feild¹; ¹Shimadzu Scientific Instr., Columbia, MD; ²NanoMedical Systems, Houston, TX

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- TP 491 **Physical Vapor Deposition Screening for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry Applied to Microbiome Metabolomics;** Rebecca Hansen¹; Maria Emilia Dueñas¹; Gargey Yagnik¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- TP 492 **The Molecular Scanner Approach: Applications in Tissue Imaging;** William Andrews¹; Merlin Bruening¹; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN
- TP 493 **Metal Organic Frameworks as a New Class of MALDI Matrices;** Rabih Jabbour¹; Gregory W. Peterson²; Jared B. Decoste²; ¹ECBC, APG, MD; ²ECBC, US Army, Gunpowder, MD
- TP 504 **Metabolomic Profiling of NGLY1 Deficiency Disease;** Songjie Chen¹; Guangwen Wang¹; David Marciano¹; Michael Snyder¹; ¹Stanford University School of Medicine, Stanford, CA
- TP 505 **Application of GC Orbitrap Mass Spectrometry for Untargeted Metabolomics of Pathogenic Microorganisms;** Fausto Pigozzo¹; Cristian Cojocariu²; Paul Silcock²; Stefan Weid³; Jeni Haggarty³; Karl Burgess³; ¹Thermo Fisher Scientific, Rodano, Milano; ²Thermo Fisher Scientific, Runcorn, UK; ³Glasgow Polyomics, University of Glasgow, Glasgow, UK
- TP 506 **Rapid Threat Analysis – A Workflow to Support Metabolomics Analysis of a Cell's Response to an Unidentified Toxin in 30 Days;** Randi Gant-branum¹; Stacy D. Sherrod²; Simona Gabriela Codreanu²; Alexandra C Schrimpe-Rutledge²; James M Poland²; Jerry Holman²; Nicole Muszynski²; James C Pino²; Carrie E. Romer²; Jamie L. Allen²; Richard M. Caprioli²; John A. McLean²; ¹Vanderbilt University, Nashville, tenn; ²Vanderbilt University, Nashville, TN



TUESDAY POSTERS

- TP 507 **Global Metabolomic Profiling Identifies Novel Mechanisms of Cuprizone-Mediated Oligodendrocyte Dysfunction**; Alexandra Taraboletti¹; Tia Walker²; Robin Avila³; He Huang¹; Joel Caporoso⁴; Erendra Manandhar¹; Thomas Leeper⁵; David Modarelli¹; Satish Medicetty³; Leah Shriver¹; ¹University of Akron, Akron, OH; ²Indiana University Northwest, Gary, IN; ³Renovo Neural, Inc., Cleveland, OH; ⁴University of Pittsburgh School of Medicine, Pittsburgh, PA; ⁵College of Wooster, Wooster, OH
- TP 508 **Evaluation of the Metabolism of Azo Dyes and its Effects on the *Staphylococcus aureus* Metabolome**; Jinchun Sun¹; Jinshan Jin²; Richard D. Beger³; Carl E. Cerniglia⁴; Huizhong Chen⁴; ¹NCTR / USFDA, Jefferson, AR; ²Division of Microbiology, Jefferson, AR; ³Division of System Biology, National Center for Toxicological Research, Jefferson, AR; ⁴Division of Microbiology, National Center for Toxicological Research, Jefferson, AR
- TP 509 **Metabolite Fragmentation in Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation**; Ziad Sahab¹; Sylwia Stopka¹; Bindesh Shrestha²; Hang Li³; Wei Yuan¹; Lida Parvin¹; Akos Vertes¹; ¹George Washington University, Washington, DC; ²Waters Corporation, Beverly, MA; ³George Washington University, Washington, DC
- TP 510 **Metabolomic Profiles of Normal Airway Epithelium Cells Upon Exposure to Cigarette Smoking Condensate**; Alexandra C Schrimpe-Rutledge^{1,2}; Xiangming Ji^{3,4}; Simona Gabriela Codreanu^{1,2}; Stacy D. Sherrod^{1,2}; Pierre D Massion^{5,6,7}; John A. McLean^{1,2,8,9}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Center for Innovative Technology, Vanderbilt University, Nashville, TN; ³Division of Allergy, Pulmonary and Critical Care Medicine, Vanderbilt University School of Medicine, Nashville, TN; ⁴Vanderbilt Ingram Comprehensive Cancer Center, Vanderbilt University School of Medicine, Nashville, TN; ⁵Division of Allergy, Pulmonary and Critical Care Medicine, Department of Medicine, Cancer Early Detection and Prevention Initiative, Vanderbilt Ingram Cancer Center, Nashville, TN; ⁶Department of Cancer Biology, Vanderbilt University Medical Center, Nashville, TN; ⁷Veterans Affairs, Tennessee Valley Healthcare System, Nashville, TN; ⁸Vanderbilt Institute of Chemical Biology, Vanderbilt University, Nashville, TN; ⁹Vanderbilt Institute for Integrative Biosystems Research and Education, Vanderbilt University, Nashville, TN
- TP 511 **A Lipidomics Characterization of Zika-Infected Mosquito Cells**; Carlos Fernando Odir Rodrigues Melo¹; Diogo Noin de Oliveira²; Estela de Oliveira Lima¹; Tatiane Melina Guerreiro¹; Cibele Zanardi Esteves¹; Rodrigo Ramos Catharino¹; ¹Innovare Biomarkers Laboratory, Campinas, Brazil
- TP 512 **High throughput Metabolomics Using FTICR-MS to Reveal Rat Exposure States to Pesticides**; Baninia Habchi^{1,2}; Sandra Alves²; Delphine Jouan-Rimbaud Bouveresse¹; Brice Appenzeller³; Douglas N. Rutledge¹; Alain Paris⁴; Estelle Rathahao-Paris¹; ¹UMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, Massy, France; ²Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; ³Human Biomonitoring Research Unit, Luxembourg Institute of Health (LIH), Rue Henri Koch 29, Esch-sur-Alzette, Luxembourg; ⁴Sorbonne Universités, Muséum national d'Histoire naturelle, CNRS, UMR7245 MCAM, Paris, France
- TP 513 **LC/MS-Based Lipidomic Profiling in Heart Tissue of Mice with Diet-Induced Atherosclerosis**; Sunhee Jung¹; Miso Nam¹; Do Hyun Ryu²; Geum-Sook Hwang¹; ¹Korea Basic Science Institute, Seoul, South Korea; ²Sungkyunkwan University, Suwon, South Korea
- TP 514 **Single-Probe MS Analysis of Extracellular Metabolites in Live *in vitro* Tumors**; Mei Sun¹; Ning Pan¹; Zhibo Yang²; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Norman, OK
- TP 515 **Profiling Strategies for Discovery of Acylated Specialized Metabolites**; Steven M. Hurney¹; Gaurav D. Moghe¹; Robert L. Last¹; A. Daniel Jones¹; ¹Michigan State University, East Lansing, MI
- TP 516 **High Throughput Metabolomics by Ion Mobility Mass Spectrometry**; Sandra Alves¹; Alain Paris²; Guillaume Van der Rest³; Estelle Rathahao-Paris⁴; ¹Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; ²Sorbonne Universités, Muséum national d'Histoire naturelle, CNRS, UMR7245 MCAM, Paris, France; ³Université Paris Sud, Laboratoire de Chimie Physique, Orsay, France; ⁴UMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, Massy, France
- TP 517 **Development of a Serum Metabolome Database Using Isotope Labeling and High-resolution LC-MS**; Wei Han¹; Minglei Zhu¹; Ngoc Tran Tran¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- TP 518 **Mass Spectrometric Investigation of the Human Gut Microbiota's Response to Infection as a Source for Novel Antibiotics**; Caitlin Keller¹; Jennifer Bratburd¹; Cameron Currie¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- TP 519 **A Metabolomics Approach to Dissecting γ-Aminobutyrate Metabolism and its Link to Virulence and Reproduction in the Wheat Pathogen *Parastagonospora nodorum***; Hayley Abbiss^{1,2,3}; Oliver Mead⁴; Susan Breen⁴; Joel P A Gummer^{1,2}; Stacey N Reinke^{1,2}; Robert D Trengove^{1,2}; Peter S Solomon⁴; ¹Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; ²Murdoch University, Perth, Western Australia; ³SpectralWorks, Runcorn, UK; ⁴Research School of Biology, The Australian National University, Canberra, Australia
- TP 520 **Modifying Skin Metabolome and Microbiome with Personal Care Products**; Amina Bouslimani¹; Ricardo Silva¹; Amnon Amir²; Tomasz Kosciolk²; Stefan Janssen²; Kathleen Dorrestein¹; Gregory Humphrey²; James Gaffney²; Tara Schwartz²; Karenina Sanders²; Alexey V Melnik¹; Chris Callewaert²; Tal Luzzatto-Knaan¹; Rob Knight^{2,3,4}; Pieter C. Dorrestein^{1,2,4,5}; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ²Department of Pediatrics, University of California San Diego, La Jolla, CA; ³Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; ⁴Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; ⁵Department of Pharmacology, University of California San Diego, La Jolla, CA
- TP 521 **Dietary Effects on the Human Urine Metabolome: A Case Study Involving Cow Milk Consumption**; Dorothea Mung¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- TP 522 **Discovery of Biomarkers of Brain Tumor Metastasis in a Medulloblastoma Mouse Model**; Danning Huang¹; Martin R. L. Paine¹; Jingbo Liu²; David A. Gaul¹; Tobey J. MacDonald²; Facundo M. Fernández¹; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; ²Aflac Cancer and Blood Disorders Center, Department of Pediatrics, Emory University School of Medicine, Atlanta, GA
- TP 523 **Using Non-Targeted High Resolution LC-QTOF Profiling to Characterize Metabolic Responses of *Nicotiana attenuata* during Infection with *Rhizophagus irregularis***; Sven Heiling¹; Ming Wang¹; Rayko Halitschke¹; Emmanuel Gaquerel²; Aiko Barsch³; Magdalen Reinkensmeier³; Ian T Baldwin¹; ¹Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany; ²Centre



- for Organismal Studies Heidelberg, University of Heidelberg, Heidelberg, Germany; ³Bruker Daltonics, Bremen, Germany
- TP 524 **Profiling of Wine Using Ultra-High Resolution Flow Injection Mass Spectrometric Analysis and 1H-NMR Spectroscopy**; Matthias Witt¹; Nikolas Kessler¹; Markus Godejohann²; Michael L. Easterling³; ¹Bruker Daltonik GmbH, Bremen, Germany; ²Bruker BioSpin GmbH, Rheinstetten, Germany; ³Bruker Daltonic, Billerica, MA
- TP 525 **An Untargeted Metabolomics Approach to Using High Resolution Mass Spectrometry for Identifying Disease Biomarkers**; GINA TAN¹; Svetlana Rezinciuc²; Heather S. Smallwood²; Andreas F. Huhmer³; ¹Thermo Fisher Scientific, San Jose, CA; ²University of Tennessee Health Science Center, Memphis, TN; ³Thermo Fisher Scientific, San Jose, CA
- TP 526 **A Metabolomics Study on crtEBI Recombinant *Saccharomyces cerevisiae* with UHPLC Tandem Quadrupole-Time of Flight Mass Spectrometry**; Wei Du¹; TAO BO¹; ¹Agilent Technologies, Beijing, China
- TP 527 **Biomarkers for Human Plasma Sample Quality Using an IROA-Labeled Universal Internal Standard**; Casey A. Chamberlain¹; Chris Beecher²; Timothy J. Garrett¹; ¹University of Florida, Gainesville, FL; ²IROA Technologies, Gainesville, FL

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- TP 528 **Surface-assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry of Small Biomolecules and Asphaltenes Using Transition Metal Oxide Nanoparticles**; Abayomi Olaitan¹; Lauren F. Barnes¹; Joseph R. Yount¹; Savanna Ward¹; Bryan Zanca¹; Karen S. Molek¹; ¹University of West Florida, Pensacola, Florida
- TP 529 **Field-Flow Fractionation (FFF) Coupled with ICP-MS for Characterization of Metallic Nanoparticles in Tattoo Ink, and FFF-splCP-MS Analysis of Gold Nanoparticles**; Robert Reed¹; Soheyl Tadjiki¹; Florian Meier²; Tony Pfaffe²; Evelin Moldenhauer²; Thorsten Klein²; ¹Postnova Analytics Inc., Salt Lake City, Utah; ²Postnova Analytics GmbH, Landsberg am Lech, Germany
- TP 530 **Temperature and pH Alteration of Silver Nanoparticle Protein Corona Composition Studied by Quantitative Label-Free Proteomics**; Vladimir Gorshkov¹; Julia A Bubis^{2,3}; Elizaveta M Solovyeva^{2,3}; Mikhail V Gorshkov^{2,3}; Frank Kjeldsen¹; ¹University of Southern Denmark, Odense, Denmark; ²V. L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; ³Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia
- TP 531 **Development of Antibody Decorated Magnetic Nanoparticles for the Assay of Abused Drug in Urine**; Kun-Ru Wu¹; He-Hsuan Hsiao¹; ¹NCHU, Department of Chemistry, Taichung, Taiwan
- TP 532 **Surface Chemistry Analysis of Bio-Conjugated Gold Nanoparticles by LDI/MALDI-(CID)-FTICR MS**; Fabrizio Chiodo^{1,2}; Yuri E.M. van der Burgt¹; Jeroen D. Codée²; Manfred Wührer¹; Cornelis H. Hokke¹; Simone Nicolardi¹; ¹Leiden University Medical Center, Leiden, Netherlands; ²Leiden University, Leiden, Netherlands
- TP 533 **Analysis of Fungal Epipolythiodioxopiperazine Alkaloids Encapsulated within Expansile Nanoparticles via UPLC-MS/MS**; Chiraz Soumia Amrine¹; Aaron H Cobly²; Mark W Grinstaff³; Joanna E Burdette³; Daniel A Todd¹; Cedric J Pearce⁴; Nicholas H Oberlies¹; ¹University of North Carolina at Greensboro, Greensboro, NC; ²Boston University, Boston, Massachusetts; ³University of Illinois, Chicago, Illinois; ⁴Mycosynthetix, Inc, Hillsborough, NC
- TP 534 **Molecular Analysis of Neurons from Single Ganglia of *Lymnaea stagnalis* by MALDI and Nanophotonic Laser Desorption Ionization Mass Spectrometry**; Nikkita Khattar¹; Linwen Zhang¹; Zita Zrinyi²; Zsolt Pirger²; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²Balaton Limnological Institute, Tihany, Hungary
- TP 535 **Analysis of Microorganism Extracts by Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays**; Jarod Fincher¹; Akos Vertes¹; ¹The George Washington University, Washington, DC
- TP 536 **Surface Modified and Derivatized Silicon Nanopost Arrays for Increased Molecular Coverage and Sensitivity by Laser Desorption Ionization Mass Spectrometry**; Jacqueline E. Dyer¹; Jarod A. Fincher¹; Rachelle S. Jacobson¹; Nicholas J. Morris²; Matthew J. Powell²; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²Protea Biosciences, Morgantown, WV

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- TP 537 **ESI and CAD MS Studies of Fe(II) Binding to RNA Mononucleotides**; Giovanni Calderisi¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Tirol
- TP 538 **TiO₂-Based Solid Phase Extraction and LC-Coupled Mass Spectrometry for the Detection of 2'-O-methylmodifications in tRNA**; Manasses Jora¹; Robert Ross¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- TP 539 **LC-MS Based Detection of Radiation Induced Effects on RNA and Its Chemical Modifications**; Congliang Sun¹; Patrick A. Limbach¹; Balasubrahmanyam Addepalli¹; ¹University of Cincinnati, Cincinnati, OH
- TP 540 **Quantitation of siRNA in Biological Matrices by Liquid Chromatography and High Resolution Accurate Mass Spectrometry (LC/MS-HRAM)**; Ju Liu¹; Krishna Aluri¹; Vikrant Gohil¹; Chris Tran¹; Jing Li¹; Samuel Wainhaus¹; Yuanxin xu¹; ¹Alnylam Pharmaceuticals, Cambridge, MA
- TP 541 **Identification of Post-Transcriptional Modifications of tRNAs in Archaeal Organisms Using Liquid Chromatography and Mass Spectrometry**; Ningxi Yu¹; Patrick A. Limbach²; ¹University of Cincinnati, Cincinnati, Ohio; ²University of Cincinnati, Cincinnati, OH
- TP 542 **Improving MS Sensitivity through the Reduction of Metal Salt Adducts in IP-RPLC/MS Oligonucleotide Analyses**; Robert Birdsall¹; Martin Gilar²; Joe Fredette²; Ying Qing Yu²; Weibin Chen²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Milford, MA
- TP 543 **Impurity Profiling Second Generation Therapeutic Oligonucleotides Using Liquid Chromatography Mass Spectrometry**; Noha Morsy ElZahar¹; Nancy Magdy²; Amira M. El-Kosasy²; Michael G. Bartlett¹; ¹Department of Pharmaceutical and Biomedical Sciences, College of Pharmacy, The University of Georgia, Athens, GA; ²Pharmaceutical Analytical Chemistry Department, Faculty of Pharmacy, Ain Shams University, Cairo, Egypt
- TP 544 **Characterization of Amino Acid-Linked Platinum Adducts to RNA via Tandem Mass Spectrometry**; Chenchen He¹; Bett Kimutai¹; Lucas A. Hamlow¹; Yanlong Zhu¹; Harrison A. Roy¹; Jun Jiang¹; Xun Bao¹; C. S. Chow¹; Jonathan Martens²; Juehan Gao²; Giel Berden²; Jos Oomens²; M. T. Rodgers¹; ¹Wayne State University, Detroit, MI; ²FELIX Facility, Radboud University, Netherlands
- TP 545 **Characterization of Post-Transcriptional Modifications Using Low-Mass-Fragment Signatures Generated by Highly-Accurate Tandem Mass Spectrometry**; Hiroshi Nakayama¹; Yuko Nobe²; Yoshio Yamauchi²; MASATO TAOKA²; Toshiaki Isobe²; ¹RIKEN Center for Sustainable Resource Science, Wako, Japan; ²Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan
- TP 546 **Characterization of Intramolecular Nucleobase-Phosphate Interactions by Site-Specific Nucleobase Methylation and Collisionally Activated Dissociation**; Heideline Glasner¹; Christian Riml¹; Christoph



TUESDAY POSTERS

- TP 547 Falschlunger¹; Ronald Micura¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Austria
Identification of a Novel Deaminated Metabolite on a Single-Stranded Oligonucleotide, in Monkey Liver by HPLC and High-Resolution Mass Spectrometry; Jing Li¹; Ju Liu¹; Samuel Wainhaus¹; Yuanxin Xu¹; ¹Alnylam Pharmaceuticals, Cambridge, MA
- TP 548 **Two Quantitative Assays for the Phosphorodiamidate Morpholino Oligomer (PMO)SRP-4045 in Mouse Plasma using HPLC-MS/MS Coupled with Solid Phase Micro-Extraction;** AIHUA LIU¹; Jiangbo Zhang²; Nan Zhao¹; Shawn Burton¹; Michael Carver²; Sherry Liu¹; Joseph Rutkowski¹; Scott Reuschel¹; Min Meng¹; ¹Covance, Salt Lake City, UT; ²Sarepta Therapeutics, Inc., Cambridge, MA
- TP 549 **Metal Ion-, Base-, and Acid-Catalyzed Hydrolysis of Total Yeast RNA for Kendrick Mass Analysis of Posttranscriptionally Modified Nucleotides;** Matthias Halper¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Austria
- TP 550 **Characterization of Metallocene-Oligonucleotide Adducts with Different Activation Techniques;** Rahel Eberle; University of Bern, Bern, Switzerland
- TP 551 **Novel Cytidine Specific Ribonuclease for MS-Based RNA Modification Mapping;** Priti Thakur¹; Patrick A. Limbach¹; Balasubrahmanyam Addepalli¹; ¹University of Cincinnati, Cincinnati, OH
- TP 552 **Untargeted Metabolomic Profiling of the Epitranscriptome: Discovery of New Modified Nucleobases in RNA;** Megan R Showalter¹; Tomas Cajka¹; Nont Kosaisawe¹; Kacey VanderVorst²; Kermit L Carraway III²; Oliver Fiehn¹; ¹NIH West Coast Metabolomics Center, University of California Davis, Davis, CA; ²Department of Biochemistry and Molecular Medicine, UC Davis, Sacramento, CA
- TP 553 **Identification of YTHDF2 as a Reader for 5-Methylcytosine in RNA;** Xiaoxia Dai¹; Lin Li¹; Jie Li²; Gwendolyn Gonzalez¹; Changjun You¹; Weili Miao¹; Junchi Hu³; Lijuan Fu¹; Yanhui Xu²; Weifeng Gu¹; Yinsheng Wang¹; ¹UC Riverside, Riverside, CA; ²Fudan University, Shanghai, China; ³Shanghai Institute of Materia Medica, Shanghai, Shanghai
- TP 554 **LC-MS/MS for the Investigation of the Altered Levels of 5-HmdC in Cancer Cells;** Yang Yu¹; Yinsheng Wang¹; ¹UC Riverside, Riverside, CA
- TP 555 **Novel Fluorescently-Labeled Nucleotide Triphosphates - Incorporation with different DNA polymerases: MALDI MS Perspective;** Igor P. Smirnov¹; Galina E Pozmogova¹; Alexandr V Chudinov²; Edward N Timofeev²; ¹Institute of Physico-Chemical Medicine, Moscow, Moscow; ²Engelhardt Institute of Molecular Biology, Moscow, Russia
- TP 556 **Evaluation of RNase U2 Variants By Mass Spectrometry for the Improvement of RNA Modification Mapping;** Beulah Mae Ann Solivio¹; Balasubrahmanyam Addepalli¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH

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- TP 557 **Investigating Protein Interactions of MALAT-1, a Long-Noncoding RNA, in Brain Tumors;** Maike Langin^{1, 2, 3}; Nan Qin^{2, 3, 4}; Daniel Picard^{2, 3, 4}; Anja Stefanski^{1, 5}; Kai Stühler^{1, 5}; Marc Remke^{2, 3, 4}; ¹Institute of Molecular Medicine, University Hospital Duesseldorf, Duesseldorf, Germany; ²Department of Pediatric Oncology, Hematology and Clinical Immunology, University Hospital Duesseldorf, Duesseldorf, Germany; ³Division of Pediatric Neuro-Oncogenomics, German Cancer Consortium and German Cancer Research Center - partner site Essen/Duesseldorf, Duesseldorf, Germany; ⁴Department of Neuropathology, Heinrich Heine

- University Duesseldorf, Duesseldorf, Germany; ⁵Molecular Proteomics Laboratory, BMFZ, Heinrich Heine University, Duesseldorf, Germany
- TP 558 **Photoaffinity Probes and Quantitative Proteomics Enable Assessment of Target Engagement and Compound Potency in Live Cells;** Christian Eberl¹; Johanna Vappiani¹; Anne J. Wagner¹; Stephanie Lehmann¹; Marcel Muelbauer¹; Marcus Banscheff¹; ¹Cellzome, Heidelberg, BW
- TP 559 **Revisiting Ethanol Precipitation of Plasma Proteins to Deplete Albumin and Increase Depth of Coverage;** Nicholas J. Carruthers¹; Paul Stemmer²; Joseph A. Caruso²; ¹Wayne State University, Detroit, MI; ²Wayne State University, Detroit, MI
- TP 560 **Alpha-Lytic Protease Digestion of Proteins: Comparison with Trypsin and Subtilisin;** Colleen McClung¹; Christopher J Noren¹; Cristian I. Ruse¹; ¹New England Biolabs, Ipswich, MA
- TP 561 **Cell Surface Thermal Proteome Profiling Enables Monitoring the Interactions of Small Molecules and Endogenous Ligands with the Plasma Membrane Proteome;** Matthias Kalxdorf¹; Ina Tögel¹; Christian Eberl¹; Marcus Bantscheff¹; ¹Cellzome, a GSK company, Heidelberg
- TP 562 **Characterization of Degradation Profile of Collagen in Archaeological Specimens by Mass Spectrometry;** Mao Karino¹; Kazuki Kawahara²; Seiji Kadowaki³; Yoko Taniguchi⁴; Akira Tsuneki⁴; Mehdi Moini⁵; Takashi Nakazawa¹; ¹Nara Women's University, Nara, Japan; ²Osaka University, Suita, Japan; ³Nagoya University Museum, Nagoya, Japan; ⁴University of Tsukuba, Tsukuba, Japan; ⁵George Washington University, Washington, DC
- TP 563 **Comparative Microsomal Proteomics of the NCI-H23 Lung Cancer Cell Line Grown in 2D and 3D Culture;** Jan A. Kaczmarczyk¹; Rhonda R. Roberts¹; Richard G. Saul¹; John J. Gildea²; Robin A. Felder³; Gordon R. Whiteley¹; Josip Blonder¹; ¹Frederick National Laboratory for Cancer Research (FNLCR), Leidos Biomedical Research Inc., Frederick, MD; ²Omic Labs, Scottsville, VA; ³Department of Pathology, University of Virginia School of Medicine, Charlottesville, VA
- TP 564 **Mass Spectrometry Based Identification, Quantitation, and Characterization of Novel Cell Surface Markers of Human Cardiomyocytes;** Matthew Waas¹; Ted Keppel¹; Chelsea Fujinaka¹; Ranjuna Weerasekera¹; Rebekah Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI
- TP 565 **Discovery and Quantitation of Cell Surface Proteins during Pluripotent Stem Cell-Derived Cardiomyocyte Differentiation and Maturation;** Chelsea Fujinaka¹; Ted Keppel¹; Matthew Waas¹; Rebekah Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI
- TP 566 **The Quantification of Low Abundance Host Cell Protein Impurities by Standard Addition Mass Spectrometry Method;** Feng Yan¹; Zihao Wang¹; ¹GSK Vaccines, Rockville, MD
- TP 567 **Protease Networks and Proteostasis in Plant Chloroplasts and Mitochondria; an Omics Approach to Organellar Protein Maturation, Stability and Turnover;** Klaas J. Van Wijk¹; Elden Rowland²; Kristina Majsec²; Giulia Friso¹; Nazmul H. Bhuiyan²; Jitae Kim²; Vivek Kumar³; Sunita Kumari³; Doreen Ware³; Qi Sun²; ¹Cornell University, Ithaca, New York; ²Cornell University, Ithaca, New York; ³Cold Spring Harbor laboratory, Cold Spring Harbor, NY
- TP 568 **Multiplexed Mass Spectrometric Screening of EGFR Mutations in Non-small-cell Lung Cancer;** Chi-Ting Lai¹; Wai-Kok Choong²; T. Mamie Lih²; Hui-Yin Chang²; Ting-Yi Sung²; Hsuan-Yu Chen³; Yu-Ju Chen⁴; Chia-Li Han⁵; ¹Genome and Systems Biology Degree Program,



National Taiwan University, Taipei, Taiwan; ²Institute of Information Science, Academia Sinica, Taipei, Taiwan; ³Institute of Statistical Science, Academia Sinica, Taipei, Taiwan; ⁴Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ⁵Master Program for Clinical Pharmacogenomics and Pharmacoproteomics, Taipei Medical University, Taipei, Taiwan

PROTEINS: PTMs
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- TP 569 **Development of a Method for the Determination of α -Tubulin Acetylation by Immunopurification-Multiple Reaction Monitoring Mass Spectrometry (IP-MRM-MS);** Xiangkun Yang¹; Michael Bartlett¹; ¹University of Georgia, Athens, Georgia
- TP 570 **2D-Immunoblotting Combined with High-Resolution Mass Spectrometry Reveals a Novel Phosphorylation Site in Cofilin-1 Involved in Cardiomyopathy;** Solenne Chardonnet¹; Maria Chatzifrangkeskou²; Yannick Tanguy²; Thibault Marais²; Howard J. Worman^{3,4}; Gisèle Bonne²; Antoine Muchir²; ¹Sorbonne Universités, UPMC Univ Paris 06, Inserm, UMS Omique, Plateforme P3S, Paris, France; ²Center of Research in Myology, UPMC-INSERM UMR974, CNRS FRE3617, Paris, France; ³Department of Medicine, College of Physicians and Surgeons, Columbia University, New York, NY; ⁴Department of Pathology and Cell Biology, College of Physicians and Surgeons, Columbia University, New York, NY
- TP 571 **Development of a High-throughput Method to Identify Disulfides in Human Recombinant Soluble Guanylyl Cyclase;** Chuanlong Cui¹; Lin Yan¹; Annie Beuve²; Hong Li¹; ¹Center for Advanced Proteomics Research, Rutgers New Jersey Medical School, Newark, NJ; ²Department of Pharmacology, Physiology and Neuroscience, Rutgers New Jersey Medical School, Newark, NJ
- TP 572 **Highly Efficient and Reproducible Online 2D-LC Method for Determination of Glycated Peptides;** Lina Zhang¹; Chih-Wei Liu¹; Qibin Zhang^{1,2}; ¹Center for Translational Biomedical Research, Kannapolis, NC; ²University of North Carolina at Greensboro, Greensboro, NC
- TP 573 **Characterization of Disulfide Linkages in Proteins by Ultraviolet Photodissociation (UVPD);** Montana Quick¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TP 574 **Reprogramming the SNO-Proteome in the brain of the Shank3-KO Model of Autism Spectrum Disorder;** Haitham Amal¹; Vadira Bhat²; John S. Wishnok¹; Guoping Feng³; Steven R. Tannenbaum^{1,3}; ¹Massachusetts Institute of Technology, Cambridge, MA; ²Agilent Technologies, Wilmington, DE; ³McGovern Institute for Brain Research, Cambridge, MA
- TP 575 **Succinyl-CoA Potentially Regulates the Oligomeric Forms of Cyanobacterial Citrate Synthase through Succinylation;** John Muroski¹; Hong Nguyen¹; Joseph A. Loo¹; Rachel R. Ogorzalek Loo¹; ¹UCLA, Los Angeles, CA
- TP 576 **Comprehensive Profiling of Lysine Modifications in Biosilica-Associated Proteome;** Alexander Milentyev¹; Christoph Heintze²; Nicole Poulsen²; Nils Kröger^{2,3}; Andrej Shevchenko¹; ¹MPI-CBG, Dresden, Germany; ²B-CUBE Center for Molecular Bioengineering, Dresden, Germany; ³Department of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany
- TP 577 **Automated Proteome-Wide Data Analysis Strategies for the "Unbiased" Detection of Dityrosine Cross-Linked Proteins Indicative of Oxidative Stress in Neurodegenerative Diseases;** Eugene A Kapp¹; Soumya Mukherjee²; Blaine R Roberts¹; ¹The Florey, Melbourne, Australia; ²Indian Association for the Cultivation of Science, Jadavpur, India
- TP 578 **Symmetric Dimethylated Arginines Residues in Proteins from Human Lung Cancer Cells;** Stephanie Lehman¹; Hongshan Chan²; Dina L Bai³; Jeffrey Shabanowitz³; Donald F Hunt³; David Shechter⁴; ¹University of Virginia, Charlottesville, VA; ²Nanjing Medical University, Nanjing, China; ³University of Virginia, Charlottesville, VA; ⁴Albert Einstein College of Medicine, New York, NY
- TP 579 **Identification and Selective Enrichment of Functional Arginine Residues Using Bio-Orthogonal Click Chemistry and Mass Spectrometry;** Maheshika S.K. Wanigasekara¹; Abu Hena M Kamal¹; Saiful M. Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- TP 580 **Proteome-Wide Acetylation Dynamics Revealed by Metabolic Labeling and Quantitative Proteomics;** Yekaterina Kori¹; Simone Sidoli¹; Zuo-Fei Yuan¹; Peder J. Lund¹; Xiaolu Zhao²; Benjamin A. Garcia¹; ¹Epigenetics Program, Department of Biochemistry and Molecular Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA; ²Wuhan University, Wuhan, China
- TP 581 **Site-specific N-Glycosylation Mapping for Glycopeptides in the Presence of Additional Unknown Post-Translational Modifications (II) by Y1 (Peptide + HexNAc) Ion;** Benlian Wang^{1,2}; David Salom^{3,4}; Krzysztof Palczewski³; Mark R. Chance^{1,2}; ¹Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; ²Department of Nutrition, Case Western Reserve University, Cleveland, OH; ³Department of Pharmacology, Case Western Reserve University, Cleveland, OH; ⁴Polgenix, Inc., Cleveland, OH
- TP 582 **Reversible Phosphorylation of the RVSF Motif in PP1 Regulatory Proteins by Aurora B Controls PP1 Docking During the Cell Cycle;** Isha Nasa^{1,2}; Scott Rusin¹; Arminja Kettenbach¹; Greg Moorhead²; ¹Department of Biochemistry, Dartmouth College, Lebanon, NH; ²University of Calgary, Calgary, AB
- TP 583 **Strategies for Enriching and Identifying the Farnesyl Peptide from Complex Sample Using Mass Spectrometry;** Zixiang Fang¹; Saiful M. Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- TP 584 **Identification of Novel E3 SUMO Ligase PIAS1 Substrates by Quantitative Proteomics;** Chongyang Li¹; Francis McManus¹; Pierre Thibault¹; ¹IRIC-Université de Montréal, Montréal, QC
- TP 585 **Dynamic Mapping of Glyco-Conjugates in Human Prefrontal Cortex via Neuroglycomics Approach Reveals Age- and Region-Specific Biosynthetic Pathway;** Jua Lee^{1,2}; Sumin Kim^{1,2}; Sureyya Ozcan³; Sabine Bahn³; Hee-Sup Shin⁴; Hyun Joo An^{1,2}; ¹Asia Glycomics Reference Site, Chungnam National University, South Korea; ²Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; ³Institute of Biotechnology, University of Cambridge, UK; ⁴Center for Cognition and Sociality, Institute for Basic Science, South Korea
- TP 586 **Top-Down Mass Spectrometry Reveals the Impact of Cardiac Tissue Handling on Myofilament Protein PTMs;** Wenxuan Cai¹; Beini Lyu²; Zachary L Hite³; Zhijie Wu³; Ziqing Lin²; Zachery R Gregorich²; Takushi Khomoto²; Ying Ge^{2,3}; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin Madison, Madison, WI; ³University of Wisconsin - Madison Department of Chemistry, Madison, WI
- TP 587 **Direct and Indirect Analysis of S-Palmitoylated Proteins in Ocular Lens by Mass Spectrometry ;** Zhen Wang¹; Kevin L. Schey²; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt University, Nashville, TN
- TP 588 **Probing the Deleterious Effects of Protein Aging by Tracking Isomerization in the Human Eye Lens;** Yana Lyon¹; Ryan R Julian²; ¹University of California, Riverside, Riverside, CA; ²UC Riverside, Riverside, CA



- TP 589 **Regulation of RNA Polymerase II Transcription Elongation by Ubiquitylation**; Sarah Peck¹; Melanie J. Fox¹; Whitney R. Smith-Kinnaman¹; Lea Morical¹; Hongyu Gao¹; Yunlong Liu¹; Amber L Mosley¹; ¹*Indiana University School of Medicine, Indianapolis, IN*
- TP 590 **Expanding OxcyscPILOT to Study SNO and S-acyl in Aging Brain**; Ryan R Dyer¹; Renā A.S. Robinson¹; ¹*University of Pittsburgh, Pittsburgh, PA*
- TP 591 **Moneyball for PTMs: The Science of Winning the Unfair Game of Functional PTM Prognostication**; Matthew P. Torres¹; Henry M Dewhurst¹; ¹*School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*
- TP 592 **Serotransferrin Glycation and Ceruloplasmin Deamidation Result in their Increased Degradation in Type 2 Diabetes**; Makan Golizeh¹; Kwangwon Lee²; Serguei Ilchenko²; Abdullah Osme²; James Bena³; Rovshan Sadygov⁴; Takhar Kasumov²; ¹*Northeast Ohio Medical University, Rootstown, Ohio*; ²*Northeast Ohio Medical University, Rootstown, Ohio*; ³*Cleveland Clinic Foundation, Cleveland, Ohio*; ⁴*University of Texas Medical Branch, Galveston, TX*
- TP 593 **Convenient Strategy for Mapping N-Glycosylation Sites Using Microwave-Assisted Acid Hydrolysis**; Cheng Ma¹; Peng George Wang²; ¹*Georgia state university, Atlanta, GA*; ²*GSU, Atlanta, GA*
- TP 594 **Elucidating the Role of Histone H4 Lysine 79 Monomethylation in Chlamydomonas reinhardtii using Top Down Mass Spectrometry and RNA interference**; Jack W Clemmensen¹; Aliyya Khan¹; Anthony T. Iavarone²; Gary H. Karpen³; James Pesavento¹; ¹*Saint Mary's College of California, Moraga, CA*; ²*QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, CA*; ³*Lawrence Berkeley National Laboratory, Berkeley, CA*
- TP 595 **Construct N-Glycan Databases for Glycoproteomics by Using a Canonical String Representation**; Xiao-Jin Zhang¹; Wen-Feng Zeng¹; Jian-Qiang Wu¹; Yang Zhang²; Ming-Qi Liu²; Pan Fang²; Peng-Yuan Yang²; Si-Min He¹; ¹*Institute of Computing Technology, Beijing, Beijing*; ²*Fudan University, Shanghai, Shanghai*
- TP 596 **Quantitative Analysis of Phosphotyrosine Signaling Reveals the Differential Mechanism of Mutated Granulocyte-Colony Stimulating Factor Receptors (G-CSFRs) Leading to Leukemia**; Pankaj Dwivedi¹; David E Muench²; Mohammad Azam²; H. Leighton Grimes²; Kenneth D Greis¹; ¹*University of Cincinnati, Cincinnati, OH*; ²*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*
- TP 597 **Mass Spectrometry-Based Analysis of an Emerging Post-Translational Modification, AMPylation, and its Role in Molecular Signaling**; Kelly Servage¹; Amanda Casey¹; Junmei Zhang¹; Kim Orth¹; ¹*UT Southwestern, Dallas, TX*
- TP 598 **Histone Epigenetic Changes in Response to Chronic Methamphetamine Abuse**; Lisa M Orr¹; Molly H Tibbs¹; Chris Bolden¹; Eric C Peterson¹; Alan J Tackett¹; ¹*University of Arkansas for Medical Sciences, Little Rock, AR*
- TP 599 **Detection of a Phosphorylated Glycine-Serine Linker in an IgG-Based Fusion Protein Using CID, EthCD, HCD, Peptide Spiking and Alkaline Phosphatase**; Bjoern Mautz¹; Oksana Tyshchuk¹; Hans Rainer Voelger¹; Claudia Ferrara Koller²; Patrick Bulau³; Hans Koll¹; Michael Molhoj¹; ¹*Roche Pharma Research and Early Development (pRED), Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany*; ²*Roche Pharma Research and Early Development (pRED), Discovery Oncology, Roche Innovation Center Zurich, Schlieren, Switzerland*; ³*Roche Pharma Technical Development Penzberg, Penzberg, Germany*
- TP 600 **Characterization of Post Translational Modifications of Light Exposed IgG1—Assay Optimization and Cross-Validation with Four Serine-Proteinases Digestions**; Yao Chen¹; Anuja Ganesan¹; Victor Vinci¹; Yunsong Li¹; ¹*COOK PHARMICA, Bloomington, IN*
- TP 601 **Charge State Distribution Modification as a Mechanism to Reduce Apparent Complexity of an Intact Fusion Protein Therapeutic**; Matthew D Maust¹; Katy Ryan¹; Heather Anderson¹; Harsha Gunawardena²; Andrew Mahan²; Eric Beil²; Hirsh Nanda²; ¹*Protea Biosciences, Morgantown, West Virginia*; ²*Janssen Pharmaceuticals R&D, Spring House, PA*
- PROTEOMICS: QUANTITATIVE II**
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- TP 602 **Discovery-Based Proteomics Identifies Molecular Signatures Associated with Hydrosalpinx**; Elizabeth Yohannes¹; Avedis Kazanjian²; Gregory Chow³; Ronald Beesley⁴; Ryan Heitmann⁵; Richard Burney^{3,5}; ¹*Department of Clinical Investigation, MADIGA Army Medical Center, 9040 Jackson Ave., Tacoma, WA*; ²*Department of Clinical Investigation, MADIGA Army Medical Center, 9040 Jackson Ave., Tacoma, WA*; ³*Department of Obstetrics and Gynecology, Division of Reproductive Endocrinology and Infertility, MADIGA Army Medical Center, 9040 Jackson Ave, Tacoma, WA*; ⁴*Department of Obstetrics and Gynecology, Division of Reproductive Endocrinology and Infertility, MADIGA Army Medical Center, 9040 Jackson Ave, Tacoma, US*; ⁵*Department of Clinical Investigation, MADIGA Army Medical Center, 9040 Jackson Ave, Tacoma, WA*
- TP 603 **Exploring Proteins Expressed Exclusively within the Inner Ear Hair Cells as Potential Drivers of Deafness**; Miguel Ramirez¹; Ann E. Hickox¹; Ann C.Y. Wong^{2,3}; Kwang Pak²; Chelsea Strojny¹; Allen F Ryan²; Jeffrey N Savas¹; ¹*Northwestern University Feinberg School of Medicine, Chicago, Illinois*; ²*University of California, San Diego, La Jolla, CA*; ³*University of New South Wales, Sydney, Australia*
- TP 604 **10-plex TMT Label-based Quantitative MS2 and MS3 Proteomic Analysis of Hypertriglyceridemia-induced Brain Microvascular Lipotoxic Injury**; Anthony W Herren¹; Tun Nyunt²; Brett S Phinney¹; John C Rutledge²; Nhin H Aung²; ¹*University of California, Davis, Genome Center, Davis, CA*; ²*University of California, Davis, School of Medicine, Internal and Cardiovascular Medicine, Davis, CA*
- TP 605 **Application of Scheduled GeLC-MRM Method for High-throughput Screening of Small GTPases Involved in Colon Cancer Metastasis**; Ming Huang¹; Yinsheng Wang¹; ¹*University of California, Riverside, CA*
- TP 606 **Hepatic Mitochondrial Dysfunction in a Mouse Model of NASH is Associated with Increased Degradation of Mitochondrial Proteins**; Kwangwon Lee¹; Abdullah Osme¹; Makan Golizeh¹; Serguei Ilchenko²; Mahbubur Rahman³; Rovshan Sadygov³; Takhar Kasumov¹; ¹*Northeast Ohio Medical University, Rootstown, Ohio*; ²*Northeast Ohio Medical University, Rootstown, Ohio*; ³*University of Texas Medical Branch, Galveston, TX*
- TP 607 **Dynamic Changes of Ca²⁺-Mediated Signalosome by Exposure to High-Glucose Dependent Short-Term Time-Course in the Nuclear Proteome of Pancreatic B-Cells**; Taewook Kang¹; Pia Jensen¹; Martin Røssel Larsen¹; ¹*Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*
- TP 608 **Changes in Mitochondrial Proteins, Metabolites, and Protein Acylation in Response to Macronutrient Stresses in the Mouse Liver**; Jesse G. Meyer¹; Natan Basisty¹; Samir Softic²; Guoxiao Wang²; BIRGIT SCHILLING¹; Christopher Newgard³; C. Ronald Kahn²;



- Bradford W Gibson^{1,4}; ¹Buck Institute for Research on Aging, Novato, CA; ²Joslin Diabetes Center, Harvard Medical School, Boston, MA; ³Sarah W. Stedman Nutrition and Metabolism Center, Duke University School of Medicine, Durham, NC; ⁴Amgen, Thousand Oaks, CA
- TP 609 **Label Free Quantitative Proteomics Analysis Reveals the Pathways Involved in Factor VIII Secretion by the Bradykinin Activated Mouse Dendritic Cells;** Cristina Clement¹; Monika Dzieciatkowska²; Antonia Follenzi³; ¹Albert Einstein College of Medicine, Bronx, NY; ²University of Colorado Denver, Denver, Colorado; ³School of Medicine, University of Piemonte Orientale, Novara, Italy
- TP 610 **Methanosarcina mazei, acetivorans, and barkeri Proteomic Responses to Different Methylophilic Substrates;** Deborah A. Jarrett¹; Farzaneh Sedighian¹; Hong Hanh Nguyen¹; Robert P. Gunsalus¹; Joseph A. Loo¹; Rachel O. Loo¹; ¹University of California, Los Angeles, Los Angeles, CA
- TP 611 **Comparative Proteomic Analysis of Charcoal-Stripped Fetal Bovine Serum Revealed Modified Insulin-Like Growth Factor Signaling Responsiveness;** CHENGJIAN TU¹; Michael Fiandalo²; Jun Li¹; Jun Qu¹; Li Tang²; James L. Mohler²; Yue Wu²; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Cancer Institute, Buffalo, NY
- TP 612 **Pulse Isotopic Labeling Analysis Revealed Temporal Dynamics of Lysine Acetylation Proteome;** Tong Zhou¹; Luke Erber¹; Yue Chen¹; ¹University of Minnesota at Twin Cities, Minneapolis, MN
- TP 613 **Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Biological and Technical Variance in Human Uterine Smooth Muscle Tissue;** Craig Ulrich¹; Christian Copley-Salem¹; David Quilici¹; Heather Burkin¹; Iain Buxton¹; Karen Schlauch¹; ¹University of Nevada, Reno, Reno, NV
- TP 614 **Quantitative Proteomic Analysis Applied to Differentiation of SH-SY5Y Human Neuroblastoma Cells as an in vitro Neuron-Like Model;** Jimmy Rodriguez¹; Aniel Sanchez²; Livia Goto-Silva³; Fábio CS Nogueira¹; Gilberto B Domont¹; Magno Junqueira¹; ¹Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; ²Lund University, Lund, Sweden; ³Instituto D'Or de Pesquisa e Ensino, Rio de Janeiro, Brazil
- TP 615 **Proteomic Profiles of H2S-regulated PTMs in Endothelial Cell under Hypoxia;** Xinggui Shen; LSU Health-Shreveport, Shreveport, LA
- TP 616 **Identifying the Roles of ARMS2 and HTRA1 in the Pathogenesis of AMD Using Quantitative Functional Proteomics;** Joel D Federspiel¹; Todd M Greco²; Pierre Jean Beltran¹; Jim Handa³; Richard Semba³; Ileana M Cristea¹; ¹Princeton University, Princeton, NJ; ²Princeton University, Princeton, NJ; ³Johns Hopkins University School of Medicine, Baltimore, MD
- TP 617 **Quantitative Discovery of the Alterations of the Human Kinome in Primary and Metastatic Melanoma Cells;** Weili Miao¹; Lei Guo¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA
- TP 618 **Analysis of Proteome Degradation Kinetics with in vitro and in vivo Models of Alzheimer's Disease;** Timothy Hark¹; Yi-Zhi Wang¹; Samuel Smukowski¹; Jeffrey N Savas¹; ¹Northwestern University, Chicago, IL
- TP 619 **Quantitative Proteomic Analysis of Cancer Cell Lines with Homozygous and Heterozygous Mutant KRAS Genotypes;** Josip Blonder¹; Benjamin Orsbum²; Gordon R. Whiteley¹; ¹Frederick National Laboratory for Cancer Research (FNLRC), Leidos Biomedical Research Inc., Frederick, MD; ²Thermo Fisher Scientific, West Palm Beach, Florida
- TP 620 **Comprehensive Analysis of Newly-Synthesized Protein Abundance Changes in Human Cells Stimulated with IGF1;** Ming Tong¹; Haopeng Xiao¹; Johanna Smeekens¹; Ronghu Wu¹; ¹Georgia Tech, Atlanta, GA
- TP 621 **Dynamics of Zebrafish Heart Regeneration Using an HPLC-ESI-MS/MS Approach;** DanJun Ma¹; Yuxi Yang²; Chengjian Tu³; Qianhu Sheng⁴; Xin Lou²; ¹dongguan University of Technology, Dongguan, China; ²Nanjing Medical University, Nanjing, China; ³Department of Pharmaceutical Sciences, University at Buffalo, State University of New York, Buffalo, NY; ⁴Department of Cancer Biology, Vanderbilt University, Nashville, TN
- TP 622 **Quantitative Analysis of Two Cancer Signaling Pathways Using Multiplex-Immunoprecipitation and Targeted Mass Spectrometry;** Bhavin Patel¹; Leigh Foster¹; Penny Jensen¹; Gregory Potts¹; Abid Haseeb¹; Kay Opperman¹; Rosa Viner²; Andreas Huhmer²; John Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, San Jose, CA
- TP 623 **A Targeted Quantitative Proteomic Approach for Profiling Guanine Nucleotide-Exchange Factors during Cancer Metastasis;** Tianyu Qi¹; Weili Miao¹; Ming Huang¹; Yinsheng Wang¹; ¹UC Riverside, Riverside, CA
- TP 624 **Analysis of Age-dependent Changes in the Proteome from Drosophila melanogaster Alzheimer's Disease Lines;** Chris Brown¹; Melissa A. Phelps²; Robert C. Eisman²; Jonathan Trinidad²; Thomas C. Kaufman²; David E Clemmer²; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- TP 625 **Relative Quantification Using TMT11plex on a Modified Q Exactive HF Mass Spectrometer;** Tabiwang N. Arrey¹; Rosa Viner²; Ryan D Bomgardner³; Eugen Damoc⁴; Markus Kellmann⁴; Thomas Moehring⁴; Alexander Harder⁴; ¹Thermo Fisher Scientific, Bremen, Bremen; ²ThermoFisher, San Jose, CA; ³ThermoFisher Scientific, Rockford, Illinois; ⁴Thermo Fisher Scientific, Bremen, Germany
- TP 626 **Development of a Novel Proteomics Approach to Investigate Cell Type-Specific Responses to Ethanol in Primary Glia and Neurons;** Jennifer Guergues¹; Ashley E. Culver-Cochran¹; Ping Zhang²; Bin Liu²; Stanley M Stevens¹; ¹University of South Florida, Tampa, FL; ²University of Florida, Gainesville, FL
- TP 627 **Global Proteome Characterization of Caenorhabditis elegans Dauer Larvae;** Asifa K Zaidi¹; Krishna Vukoti¹; Masaru Miyagi¹; ¹Case Western Reserve University, Cleveland, OH
- TP 628 **Global Analysis of Secreted Proteins and Glycoproteins in Saccharomyces cerevisiae;** Johanna Smeekens¹; Haopeng Xiao¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- TP 629 **Unbiased Discovery and Functional Confirmation of a Novel Target (DPP3) by Thermal Stability Label-Free Differential Mass Spectrometry (dMS);** Steven Mullett¹; Harris Bell-Temin²; Bennett Van Houten²; Wei Qian²; Andrey Bondarenko³; Mark Schurdak⁴; D. Lansing Taylor⁴; Andrew Stern⁴; Nathan A Yates²; ¹University Of Pittsburgh, Pittsburgh, Pennsylvania; ²University of Pittsburgh School of Medicine, Pittsburgh, PA; ³Infoclinika, Seattle, WA; ⁴Drug Discovery Institute, Pittsburgh, PA
- TP 630 **To TMT or LFIQ, that is here the Question;** Jane M Liu¹; Michael J Sweredoski²; Annie Moradian²; Sonja Hess²; ¹Pomona College, Pomona, CA; ²California Institute of Technology, Pasadena, CA
- TP 631 **Targeted Proteomics of Key Regulators of All-Trans Retinoic Acid During SIV Infection;** Wenjing Li¹; Jianshi Yu¹; Neil Sidell²; Maureen A Kane¹; ¹University of Maryland, Baltimore, Maryland; ²Emory University, Atlanta, Georgia
- TP 632 **Strategies in Proteomic Quantification Using Isobaric Labeling: Insights from the Partiality of MS2 Reporter-ion Ratios;** Qiang Zhang¹; Petra Erdmann-Gilmore¹; Yiling Mi²; Rose Connors²; Sherri R. Davies²; Shunqiang Li²; Reid Townsend²; ¹Washington University School of Medicine, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO



TUESDAY POSTERS

- TP 633 **A Novel Cholesterol Mimetic Activity Based Proteomic Profiling (ABPP) Probe to Validate ROR γ t-LBD Target Engagement;** Aruna B. Wijeratne¹; Jose M. Minguez¹; Christian A. Clarke¹; Timothy I. Richardson¹; Thomas A. Engler¹; Chalmers J. Michael¹; ¹Eli Lilly and Company, Indianapolis, IN
- TP 634 **Pushing the Limits: Boosting Sensitivity of PRM Assays for the Detection of Very Low Abundant Proteins in Complex Samples;** Emmanuelle Lezan¹; Erik Ahrné¹; Thomas Bock¹; Alexander Schmidt¹; ¹PCF-Biozentrum-University of Basel, Basel, Switzerland
- TP 635 **MRM and PRM Assay Development for a Panel of >3,000 Proteins from 20 Mouse Tissues;** Sarah A. Michaud¹; Nicholas J.T. Sinclair¹; Ingo Feldmann²; Yassene Mohammed^{1,3}; Derek S. Smith¹; Albert Sickmann²; Christoph H. Borchers^{1,4}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC; ²Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; ³Center for Proteomics and Metabolomics, Leiden University, Netherlands; ⁴Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC
- TP 636 **Sequential Enrichment and Quantification of Phosphorylation on Reversibly Oxidized Proteoforms in *Chlamydomonas reinhardtii*;** Leslie M. Hicks¹; Evan W. McConnell¹; Emily G. Werth¹; ¹UNC - Chapel Hill, Chapel Hill, NC
- TP 637 **Rapid and Accurate Instrumental Performance Gauge: Isotopologue Standards for Quality Control of LC-MS Platforms;** Alvaro Sebastian Vaca Jacome¹; Gauthier Husson¹; Alain Van Dorsselaer¹; Christine Carapito¹; ¹IPHC, UoS, CNRS, UMR7178, Strasbourg, France
- TP 638 **Label Free Quantitative Proteomics Using Peptide Isotope Peak Intensities in Mass Spectrometry and Comparison of Label Free Methods;** Ki Na Yun^{1,2}; Gun Wook Park¹; Ju Yeon Lee¹; Eun Sun Ji¹; Mee Jung Han³; Han Bin Oh²; Jong Shin Yoo¹; Jin Young Kim¹; ¹Biomedical Omics Group, Korea Basic Science Institute, Ochang-eup, Cheongwon-gu, South Korea; ²Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, South Korea; ³Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, South Korea
- TP 639 **Quantitative Proteomics Comparison of Individual vs Pooled Biological Replicates;** Deanna Plubell¹; Phillip A. Wilmarth¹; Ashok P. Reddy¹; Alexandra M. Fenton¹; Jessica Minnier¹; Larry L. David¹; Nathalie Pamir¹; ¹Oregon Health & Science University, Portland, OR
- TP 640 **Activity-Based Profiling of Phosphoprotein Phosphatases by Mass Spectrometry-Based Proteomics;** Scott P. Lyons¹; Isha Nasa¹; Greg Moorhead²; Arminja Kettenbach^{1,3}; ¹Department of Biochemistry and Cell Biology, Dartmouth College, Lebanon, NH; ²University of Calgary, Calgary, AB; ³Norris Cotton Cancer Center, Lebanon, NH
- TP 641 **Overclocking Multiplexed Proteomics: Millisecond Real-Time Searching Enables Data-Directed Quantitation;** Brian K Erickson¹; Christopher Rose¹; Julian Mintseris¹; Derek Bailey²; Joao A Paulo¹; Graeme McAlister²; Aleksandr Gaun¹; Vlad Zabrouskov²; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA; ²Thermo Fisher Scientific, San Jose, CA
- TP 642 **Benchmarking Proteome Quantitation: Measuring the Small Writ Large;** Jeremy O'Connell¹; Joao Paulo¹; Jonathon O'Brien¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA
- TP 643 **Multidimensional Tracking of GPCR Signaling via Peroxidase-Catalyzed (APEX) Proximity Labeling;** Marian Kalocsay¹; Jaeho Paek¹; Joao A Paulo²; Andrew Kruse¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA; ²Harvard Medical School, Boston, MA
- TP 644 **A Quantitative Method for the Comparison of Mass Spectrometer Performance;** Sandra Spencer¹; Eric Huang²; Neloni Wijeratne²; Oleg Silivra²; Claudia Martins²; Mary Blackburn²; Michael J MacCoss¹; ¹University of Washington Genome Sciences, Seattle, WA; ²ThermoFisher, San Jose, CA
- TP 645 **There Are No Absolutes, Particularly in Protein Quantification;** Patricia L. Holland¹; James J. Walters²; Kevin Ray²; Uma Sreenivasan³; Sarah Aijaz³; Russell P. Grant¹; Christopher M. Shuford¹; ¹Laboratory Corporation of America, Burlington, NC; ²MilliporeSigma, St. Louis, MO; ³MilliporeSigma, Round Rock, TX
- TP 646 **Implementation of a Surrogate Cerebrospinal Fluid for use in Quantitative LC-MS Analysis of Monoclonal Antibodies against Neurodegenerative Disorders;** Jens Rose Fogh^{1,2}; Anne-Marie Jacobsen¹; Kasper D Rand²; Line R. Olsen¹; ¹H. Lundbeck A/S, Valby, Denmark; ²Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark
- TP 647 **Development and Validation of a LC-SRM Method for Simultaneous Quantification of α , β -Tubulin Isoforms in Microtubules from Various Cell Types;** Christine Schaeffer-Reiss¹; Agnès Hovasse¹; Alain Van Dorsselaer¹; Maria M. Magiera²; Carsten Janke²; Morgane Batzenschlager³; Catherine Strassel³; François Lanza³; ¹IPHC, UoS, CNRS, UMR7178, Strasbourg, France; ²Institut Curie, Paris Orsay, France; ³UMR_S 949 Inserm, EFS-Grand Est, Université de Strasbourg, Strasbourg, France
- TP 648 **Standardizing and Harmonizing Multiple TripleTOF® Systems for DDA and DIA Using a Dedicated Performance Kit;** Nicholas Morrice¹; Tom Knapman²; Hunter Christie³; Robert Graham⁴; Julie Brazzatti⁴; Anthony Whetton⁴; ¹Sciex, Warrington, Cheshire; ²SCIEX, Warrington, UK; ³SCIEX, Redwood City, CA; ⁴University of Manchester, Manchester, UK
- TP 649 **High Throughput Microflow LC-MS/MS for High Sensitivity Peptide Quantitation in Targeted Assays;** Remco van Soest¹; Christie Hunter¹; Morty Razavi²; ¹SCIEX, Redwood City, CA; ²SISCAPA Assay Technologies, Victoria, BC
- TP 650 **Implementation of Real-Time Update for Time Scheduled Targeted Peptide Quantification (PRM) on a new Quadrupole Orbitrap Benchtop Mass Spectrometer;** Christian Thoeing¹; Sebastien Gallien²; Tabiwan Arrey¹; Kerstin Strupat¹; Yue Xuan¹; Oliver Lange¹; Markus Kellmann¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, Courtaboeuf, France
- TP 651 **Towards Comprehensive Signaling Pathway Monitoring Using Advanced PRM Methods;** Sebastien Gallien¹; Yue Xuan²; Shouling Xu³; Markus Kellmann²; Bhavin Patel⁴; John C. Rogers⁴; Alexander Harder²; Andreas F. Huhmer⁵; Ken Miller⁵; ¹Thermo Fisher Scientific, Courtaboeuf, France; ²Thermo Fisher Scientific, Bremen, Germany; ³Carnegie Institution for Science, Stanford, CA; ⁴Thermo Fisher Scientific, Rockford, IL; ⁵Thermo Fisher Scientific, San Jose, CA
- TP 652 **Endogenous AP-MS to Define the Huwe1 Interactome;** Katelyn Cassidy¹; Scott A Gerber¹; ¹Dartmouth College, Lebanon, NH



PROTEOMICS: TOP DOWN ANALYSIS II
653 - 679

- TP 653 **Assessment of the Noncovalent Interaction between FGF-2 and Glycosaminoglycans by Chip-Nanoelectrospray High Resolution Mass Spectrometry;** Adrian-Cristian Robu¹; Laurentiu Popescu^{1,2}; Daniela G. Seidler³; Alina D. Zamfir¹; ¹National Institute for Research and Development in Electrochemistry and Condensed Matter, Plautius Andronescu Str. 1, RO-300224, Timisoara, Romania; ²Faculty of Physics, West University of Timisoara, Blvd. Vasile Parvan 4, RO-300223, Timisoara, Romania; ³Hannover Medical School, Dept. of Gastroentero-, Hepato- and Endocrinology I3, EB2/R3110, Carl-Neuberg-Str. 1, D-30625, Hannover, Germany
- TP 654 **Statistical Fragmentation Pattern Discovery of Intact Proteins Based on their Large-Scale Top-down MS/MS Spectra;** Ruixiang Sun^{1,2}; Ruimin Wang²; Hao Chi²; Chao Liu²; Simin He²; Ying Ge¹; ¹University of Wisconsin, Madison, WI; ²Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China
- TP 654 **Statistical Fragmentation Pattern Discovery of Intact Proteins Based on their Large-Scale Top-Down MS/MS Spectra;** Ruixiang Sun^{1,2}; Ruimin Wang²; Hao Chi²; Chao Liu²; Simin He²; Ying Ge¹; ¹University of Wisconsin, Madison, WI; ²Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China
- TP 655 **Deciphering the Ubiquitin Code. Top-Down Analysis of Proteins Conjugated with Ubiquitin (Branched Proteins);** Fabio Gomes¹; Dapeng Chen¹; Sitara Chauhan¹; Dulith Abeykoon¹; Yan Wang²; David Fushman¹; Catherine Fenselau¹; ¹Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742; ²Proteomic Core Facility, University of Maryland, College Park, MD 20742
- TP 656 **Analysis of Myofilament Proteins from Skeletal Muscle Fibers by Top-Down Mass Spectrometry;** Yutong Jin¹; Ziqing Lin¹; Gary Diffie¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI
- TP 657 **Improving High-Throughput Top-Down Proteomics Using a Modified Hybrid Quadrupole-Ultra-High-Field-Orbitrap Mass Spectrometer;** Eugen Damoc¹; Kyle L. Fort²; Michiel van de Waterbeemd²; Christian Thoeing¹; Erik Cousijn¹; Tabiwang Arrey¹; Alexander Harder¹; Albert J. R. Heck²; Alexander Makarov¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²Utrecht University, Utrecht, Netherlands
- TP 658 **Coupling Reversed Phase Liquid Chromatography and Capillary Zone Electrophoresis for Top-Down Mass Spectrometry;** Lushuang Huang¹; Zhe Wang¹; Hongyan Ma¹; Si Wu¹; ¹University of Oklahoma, Norman, OK
- TP 659 **Mass Measurement Accuracy in Top-Down Protein Identification: Current Limits and Future Prospects;** Christopher L. Hendrickson^{1,2}; Lissa C. Anderson¹; Greg T. Blakney¹; Yuri E. Corilo¹; Lidong He²; Tingting Jiang²; Alan G. Marshall^{1,2}; Donald F. Smith¹; Chad R. Weisbrod¹; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ²Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL
- TP 660 **A Robust Top-down LC/MS-Based Proteomics Platform for Simultaneous Quantification of Protein Expression and Modifications;** Ziqing Lin¹; Liming Wei^{1,2}; Wenxuan Cai¹; Wei Guo³; Stephen P. Ford³; Gary M. Diffie¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²Fudan University, Shanghai, China; ³University of Wyoming, Laramie, WY
- TP 661 **DRY Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement in Top-Down Proteomics;** Alex Jonke¹; Jung Lee²; Peter Kottke²; David C. Muddiman³; Andrei G. Fedorov²; Matthew P. Torres¹; ¹School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA; ²George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA; ³Department of Chemistry, North Carolina State University, Raleigh, NC
- TP 662 **Multiplexing FTMS Data Analysis Workflow Improves Downstream Top-Down Structural Characterization of Proteins;** Natalia Gasilova¹; Konstantin O. Nagornov²; Kristina Srzentic³; Anton N. Kozhinov²; Yuri O. Tsybin²; Hubert H. Girault¹; ¹EPFL Valais, Sion, Valais; ²Spectroswiss Sàrl, Lausanne, Switzerland; ³Northwestern University, Evanston, IL
- TP 663 **A User-Friendly Bioinformatics Platform for Automated Continuous Elution Proteoform Analysis;** Casey E. Wing¹; John R. Corbett^{1,2}; William S. Phipps¹; Daniel A. Plymire¹; Steven M. Patrie^{1,2}; ¹University of Texas Southwestern Medical Center, Dallas, TX; ²University of Texas at Dallas, Richardson, TX
- TP 664 **Fixed Charge Chemical Modifications for Enhanced Sequencing of Native-Like Proteins and Protein Complexes;** Daniel Polasky¹; Philip C. Andrews^{2,3}; Brandon T. Ruotolo²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, MI; ³University of Michigan Medical School, Ann Arbor, MI
- TP 665 **Charge State Analysis of Native, Denatured, and Carbamylated Proteins by UVPD;** Aarti Bashyal¹; Sylvester M. Greer¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TP 666 **Quantitative Analysis of Free Circulating Light Chains Using a Tribrid Mass Spectrometer and Advanced Bioinformatics;** Moshe Gatt¹; Alexandra Gabashvili²; David Morgenstern²; Yishai Levin³; ¹Hadassah Medical Center, Jerusalem, Israel; ²Weizmann Institute of Science, Rehovot, Rehovot; ³Weizmann Institute of Science, Rehovot
- TP 667 **Capillary Electrophoresis – Mass Spectrometry for Intact Mass Analysis of Antibodies and Antibody-Drug-Conjugates;** Aran Paulus¹; Chien-Hsun Chen²; Andreas Krupke³; Stephane Houel²; Daniel Lopez Ferrer⁴; Michael Wenz³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, South San Francisco, CA; ⁴Thermo Fisher Scientific, San Jose, California
- TP 668 **Autoantibody Biomarker Discovery by Top-Down Proteomics of Serum from Patients with Systemic Lupus erythematosus;** Zhe Wang¹; Xiaowen Liu²; Kenneth Smith³; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³Oklahoma Medical Research Foundation, Oklahoma City, OK
- TP 669 **de novo Sequencing of Proteins by Top-Down 193 nm Ultraviolet Photodissociation Mass Spectrometry;** Kira Vyatkina^{1,2}; Jared B. Shaw³; Ljiljana Pasa-Tolic³; ¹Saint Petersburg State University, St Petersburg, Russia; ²SPb Academic University, St Petersburg, Russia; ³Pacific Northwest National Laboratory, Richland, WA
- TP 670 **Characterization and Quantitation of Tumor-Specific KRAS Proteoforms in Clinical Samples of Colon Cancer by Translational Top-Down Proteomics;** Ioanna Ntai¹; Luca Fornelli¹; Josiah Hutton¹; Ryan T. Fellers¹; Gordon R. Whiteley^{2,3}; Emily Boja^{2,3}; Henry Rodriguez^{2,3}; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²NIH, Bethesda, MD; ³National Cancer Institute, Bethesda, MD
- TP 671 **Analysis of Intact Hemoglobin Subunits with Ion Parking for Primary Structure Characterization;** Elizabeth Duselis¹; Jane Yang²; Scott Ugrin¹; Dina L. Bai¹; Jeffrey Shabanowitz¹; David Herold²; Donald F. Hunt¹; ¹University of Virginia, Charlottesville, VA; ²University of California, San Diego, La Jolla, CA



TUESDAY POSTERS

- TP 672 **MASH Explorer, a Universal Software Environment for Top-Down Proteomics**; Zhijie Wu¹; Sean McIlwain¹; Wenxuan Cai¹; Huseyin Guner¹; Irene M. Ong¹; Yiwen Gu¹; Sudharshanan Govindaraj Ramanathan¹; Xiaowen Liu²; Ruixiang Sun³; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³Chinese Academy of Science, Beijing, China
- TP 673 **Comparative Label-Free Quantitation of Mouse Brain Tissue Proteoforms Using Top-Down Proteomics**; Hae-Min Park¹; Roderick G. Davis¹; Ryan T. Fellers¹; Joseph B. Greer¹; Elena V. Romanova²; Stanislav S. Rubakhin²; Richard D. LeDuc¹; Paul M. Thomas¹; Justin S. Rhodes²; Jonathan V. Sweedler²; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- TP 674 **Expanding Proteoform Identifications by Constructing Proteoform Families from Intact-Mass Measurements in Top-Down Proteomic Data**; Leah V. Schaffer¹; Michael R. Shortreed¹; Anthony J. Cesnik¹; Brian L. Frey¹; Stefan K. Solntsev¹; Mark Scalf¹; Lloyd M. Smith¹; ¹University of Wisconsin Madison, Madison, WI
- TP 675 **Proteoform Dynamics**; Tao Wang¹; Mathew V. Holt¹; Nicolas Leon Young¹; ¹Baylor College of Medicine, Houston, TX
- TP 676 **Validation of Chagas' Disease Serum Biomarkers by Intact Proteins Analysis**; Elizabeth Ruiz Lancheros¹; Pierre-Olivier Schmit²; Eric Chatelain³; Jaime Althech⁴; Momar Ndao¹; ¹Research Institute - McGill University Health Centre, Montreal, Qc; ²Bruker Daltonics, Strasbourg, France; ³Drugs for Neglected Diseases initiative (DNDi), Geneva, Switzerland; ⁴Hospital de Niños Dr. Ricardo Gutierrez, Buenos Aires, Argentina
- TP 677 **In-Depth Characterization of Intact Protein Standards Using HRAM Top Down Mass Spectrometry with Multiple MSMS Strategies**; Romain Huguet¹; Helene Cardasis¹; Christopher Mullen¹; Stephane Houel¹; Luca Forneli²; Rosa Viner¹; Viktorija Vitkovsk³; Shanhua L. Lin⁴; Seema Sharma⁴; Vlad Zabrouskov¹; Neil L. Kelleher²; ¹Thermo Fisher Scientific, San Jose, CA; ²Northwestern University-Kelleher Research Group, Evanston, IL; ³Thermo Fisher Scientific, Vilnius, LT; ⁴Thermo Fisher Scientific, Sunnyvale, CA
- TP 678 **Quantitative, Localized Analysis of Mouse Brain Subregions by Top-Down Proteomics**; Roderick G. Davis¹; Hae-Min Park²; Paul M. Thomas²; Ryan T. Fellers²; Joseph B. Greer²; Richard D. LeDuc²; Amy W. Lasek³; Rosalba Satt³; Jonathan V. Sweedler⁴; Elena V. Romanova⁴; Stanislav Rubakhin⁴; Neil L. Kelleher²; ¹Northwestern University, Evanston, IL; ²Northwestern University, Evanston, IL; ³University of Illinois at Chicago, Chicago, IL; ⁴University of Illinois at Urbana-Champaign, Urbana, IL
- TP 679 **Top-Down Proteomic Analysis with Capillary Zone Electrophoresis-Mass Spectrometry**; Robert N. O'meally¹; Simion Kreimer¹; Robert N. Cole¹; ¹Mass Spectrometry and Proteomics Facility, Johns Hopkins School of Medicine, Baltimore, MD
- SMALL MOLECULES: QUALITATIVE ANALYSIS**
680 - 705
- TP 680 **Elimination of Toluene during Collision-Induced Fragmentation of Deprotonated N,N'-Diphenylacetyl dapsone Generated by Negative-Ion Electrospray Ionization Mass Spectrometry**; Chongming Liu¹; Athula Attygalle¹; ¹Stevens Institute of Technology, Hoboken, NJ
- TP 681 **Targeted Determination of Lipid Mediators in Mice Muscle Tissues Using Restricted Access Media-Based Pretreatment and Liquid Chromatography-Mass Spectrometry**; Zhiying Wang¹; Liangqiao Bian²; Chenglin Mo¹; Maciej Kukula³; Kevin A. Schug⁴; Marco Brotto¹; ¹College of Nursing and Health Innovation, The University of Texas at Arlington, Arlington, TX 76019; ²SCAAC, University of Texas at Arlington, Arlington, TX 76019; ³SCAAC, UT Arlington, Arlington, TX 76019; ⁴Departments of chemistry and biochemistry, UT Arlington, Arlington, TX
- TP 682 **Quantitative Measurement of Unconjugated Phenylephrine in Human Plasma via UHPLC with Tandem Mass Spectrometry**; Jingduan Chi¹; Yonghua Ling¹; Rand Jenkins²; Fumin Li¹; ¹PPD Inc, Madison, WI; ²PPD Inc, Richmond, VA
- TP 683 **Challenges Developing Sensitive Quantitative Assays for Cyclophosphamide and 4-Hydroxycyclophosphamide in Human Plasma Using HPLC-MS/MS**; Aihua Liu¹; Lijuan Fu¹; Qian Guo¹; Bryce Ashby¹; Scott Reuschel¹; Min Meng¹; ¹Covance, Salt Lake City, UT
- TP 684 **Development and Validation of an LC-MS/MS Method for the Quantitation of Plerixafor in Human Plasma and Urine**; Hui Hong¹; Dawei Zhou²; Baomin Xin¹; Xinping Fang²; Xin Zhang¹; ¹WuXi AppTec (Shanghai) Co. Ltd, Shanghai, China; ²WuXi AppTec. Inc, Plainsboro Township, NJ
- TP 685 **Elimination of Endogenous Light-Sensitive Compounds in Human Plasma by UV-Irradiation for the Determination of Tretinoin and Isotretinoin by LC-MS/MS**; Romain Beauvois¹; Milton Furtado¹; Anahita Keyhani¹; ¹Altasciences, Laval, QC
- TP 686 **Identification Criteria for the Analysis of Biomarkers of Chemical Warfare Agents**; R.V.S. Murty Mamidanna; Organisation for the Prohibition of Chemical Weapons, The Hague, Netherlands
- TP 687 **Elimination of Ionization Suppressing Dosing Excipient from LC-MS Method for Bendamustine and M3 in Human Plasma**; Theodore Brus; Covance, Indianapolis, IN
- TP 688 **Quantitation of Lidocaine and Its Metabolites in Human Plasma**; Adrian Bott¹; Tim Shoafr²; ¹BASi, West Lafayette, IN; ²BASi, West Lafayette, IN
- TP 689 **Analysis of Extractable and Leachable (E&L) Compounds Using a Novel Low-Energy EI Capable High Resolution Accurate Mass GC/Q-TOF**; Kevin Rowland¹; Mark Jordi¹; Kai Chen²; Jennifer Sanderson²; ¹Jordi Labs, Mansfield, MA; ²Agilent Technologies, Santa Clara, CA
- TP 690 **Extractable Study of a Drug Delivery Device - Vaginal Rings**; Li Xu¹; John Iannone¹; Wei Zhang¹; Kate Comstock²; Ekong Bassey³; John Schmelzel³; Tom Carrell³; ¹AMRI, Albany, NY; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA
- TP 691 **Extractables Analysis of Pharmaceutical Container/Packaging Labels**; John Iannone¹; Li Xu¹; Wei Zhang¹; Kate Comstock²; Ekong Bassey³; John Schmelzel⁴; Tom Carrell⁴; ¹AMRI, Albany, NY; ²Thermo Fisher Scientific, San Jose, CA; ³ThermoFisher, San Jose, CA; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 692 **Fragmentation Patterns in the Mass Spectra of Fentanyl-Type Compounds**; Kirill Tretyakov¹; Edward White V¹; Stephen Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD
- TP 693 **LC/MS/MS Method Validation for the Determination of Methamphetamine Enantiomers in Human Urine Utilizing a Novel Production Friendly Chiral Column**; Amber Awad¹; Ana Celia Grenier Ph.D¹; Lawrence J. Andrade¹; ¹Dominion Diagnostics, North Kingstown, RI
- TP 694 **Development and Validation of a Simple & Rugged LC-MS/MS Method for Determination of Unbound and Total Tiopronin in Human Plasma**; Ben Gaboury¹; Nick Peng¹; Ardeshir Khadang¹; ¹Axis Clinicals, Dilworth, MN

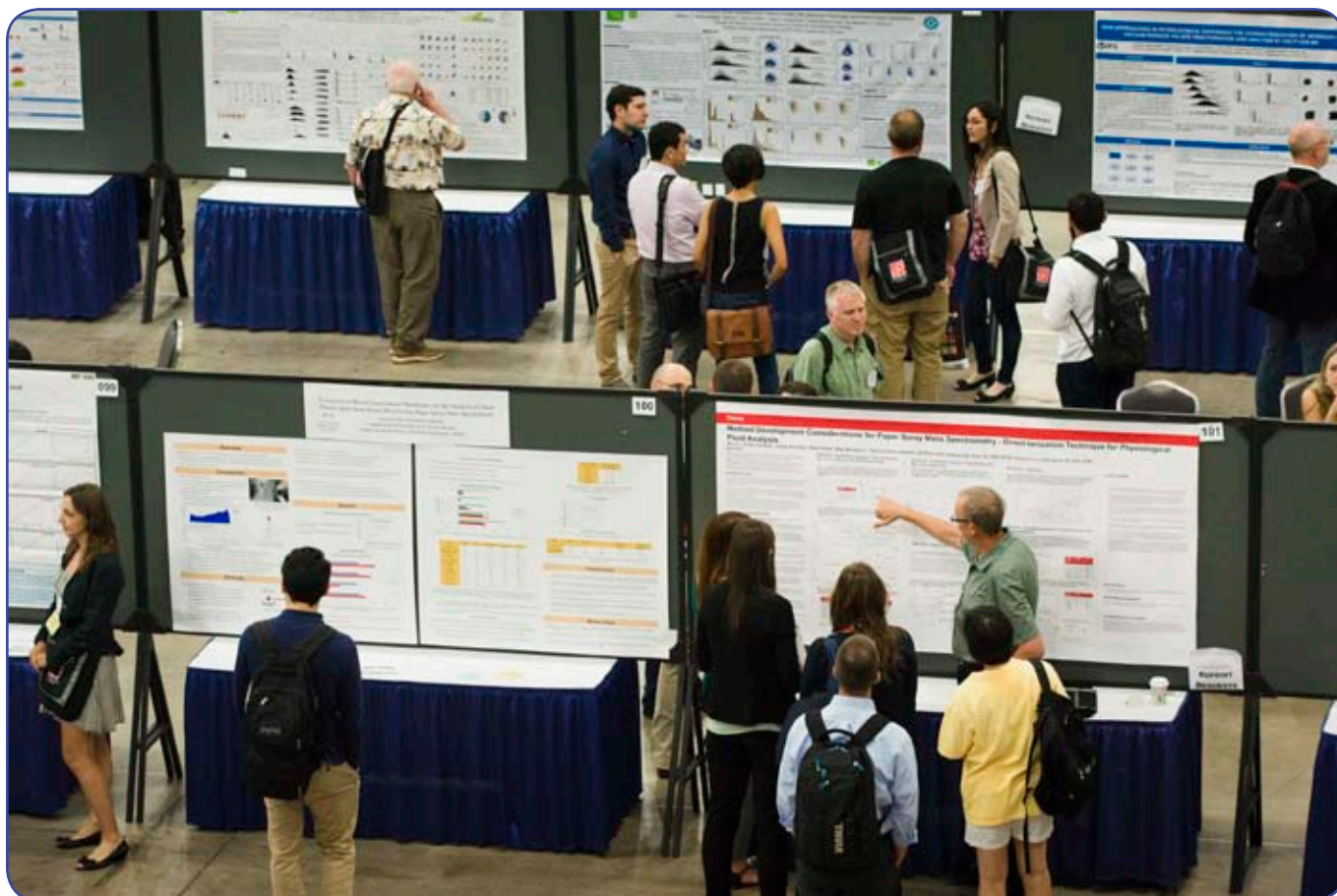


- TP 695 **Development and Validation of a Sensitive and Rugged LC-MS/MS Method to Measure Phenylephrine and Chlorpheniramine in Human Plasma;** Nick Peng¹; Ben Gaboury¹; Ardeshr Khadang¹; ¹*Axis Clinicals, Dilworth, MN*
- TP 696 **Non-Targeted Characterization of Low Molecular Weight Organic Matter along Alaskan Soil Depth Profile Using RP and HILIC Coupled with nano-ESI-HRMS/MS;** Mallory P Ladd¹; Colleen M Iversen^{1,2}; Stan D Wullschlegel^{2,3}; Shawn R Campagna⁴; Robert L Hettich^{1,5}; ¹*Bredesen Center for Interdisciplinary Research and Graduate Education, Knoxville, TN*; ²*Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN*; ³*Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*; ⁴*Department of Chemistry, University of Tennessee, Knoxville, TN*; ⁵*Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 697 **Stability Evaluation of Captopril in Human Blood by LC-MS/MS;** Eugenie Raphaelle Bérubé¹; Milton Furtado¹; Anahita Keyhani¹; ¹*Altasciences, Laval, QC*
- TP 698 **An LC-MS Screening Platform to Simultaneously Detect Clinically Relevant Antibiotics in Cholera Patient Urine and Stool;** Ludmila Alexandrova¹; Allis Chien¹; Vasavi Ramachandran²; Paul Bollyky³; Eric Nelson^{2,4}; ¹*Stanford University Mass spectrometry, Stanford, CA*; ²*Department of Pediatrics, Stanford, CA*; ³*Department of Medicine, Stanford, CA*; ⁴*Emerging Pathogens Institute, Department of Pediatrics, University of Florida, Gainesville, FL*
- TP 699 **Characterization of Industrial Amine-Based UVC Products by Chromatography-Mass Spectrometry (GC/GCMS, LC/LCMS) for REACH Registration;** Dale A. Willcox¹; Steve E. Deppen¹; Kelli L. Magarelli¹; Noelle M. Elliott¹; ¹*Intertek Allentown, Allentown, PA*
- TP 700 **Towards Quantitative Analysis without Standards: Chromatographic Retention Time as a Predictor of Mass Spectrometric Response Factor;** Daniel Foil¹; Nadja B. Cech¹; Daniel A Todd¹; ¹*University of North Carolina at Greensboro, Greensboro, NC*
- TP 701 **Multi-Class, High-Throughput Analysis of Drugs in Equine Urine and Blood by Liquid Chromatography-High Resolution Accurate Mass Spectrometry for Racing Regulation;** Efthimia Papastavros¹; Kenneth P. Matuszak²; David J. Borts¹; ¹*Iowa State University, Ames, Iowa*; ²*Thermo Fisher Scientific, Bannockburn, IL*
- TP 702 **Spatially Resolved, Quantitative Analysis of Small Molecules in Tissue Using A Laser Capture Microdissection (LCM)-LC/MS Platform;** Chengqi Hu¹; Jamie Erickson²; Youngjae Kim²; Soumya Mitra²; Stephanie Gaudette²; Annette Schwartz Sterman²; David Duignan²; Edit Tarcsa²; ¹*AbbVie, Worcester, MA*; ²*AbbVie, Worcester, MA*
- TP 703 **UVPD as a Unique Fragmentation Tool for Complete Structure Determination and Substructure Identification of Small Molecules;** Romain Huguet¹; Seema Sharma¹; Christopher Mullen¹; Jesse Canterbury¹; Mark Berhow²; Vlad Zabrouskov¹; Tim J. Stratton¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*USDA, ARS, NCAUR, Peoria, IL*
- TP 704 **Generation of an Electronic Cigarette Liquid Profile Library Using GCQTOFMS and Chromatographic Deconvolution and Comparison Software to Screen for Additives;** Hayley Abbiss^{1,2,3}; John H Moncur¹; Scott J Campbell¹; Robert D Trengove^{2,3}; ¹*SpectralWorks, Runcorn, UK*; ²*Murdoch University, Perth, Western Australia*; ³*Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia*
- TP 705 **A Comparison of the Reactivity of Para-Benzynes in Gas Phase and Solution;** Rashmi Kumar¹; Hilka Kenttamaa²; ¹*Purdue University, West Lafayette, Indiana*; ²*Purdue University-Department of Chemistry, West Lafayette, IN*
- SMALL MOLECULES: QUANTITATIVE ANALYSIS II**
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- TP 706 **Long-Term Monitoring of di-(2-Ethylhexyl)Phthalate (DEHP) Exposure in Hair Using On Line Solid Phase Extraction and Liquid Chromatography Tandem Mass Spectrometry;** Yan Zin Chang; *Taichung, Taiwan*
- TP 707 **An LC-MS/MS Method Improvement and Validation for Determination of Yeliva in Rat and Dog Plasma;** Xiaodong Shen¹; Xiao Ming Gan¹; Rwaidda Al-Eryani¹; Sridhar Korasikha¹; Sangeeta Rajasingam¹; Alain Guimond²; Reza Fathi³; Gary Johnson¹; ¹*ITR Laboratories, Montreal, QC*; ²*Insymbiosis, Montreal, QC*; ³*RedHill Biopharm Ltd., Tel Aviv, Israel*
- TP 708 **Simultaneous Determination of Sugar Phosphates in Cancer Cells by Capillary Electrophoresis-Mass Spectrometry;** Miso Nam^{1,2}; Sunhee Jung^{1,2}; Do Hyun Ryu¹; Geum-Sook Hwang²; ¹*Sungkyunkwan University, Suwon, South Korea*; ²*Korea Basic Science Institute, Seoul, South Korea*
- TP 709 **Versatile Strategies for Analysis of Sulfonate Ester Related Genotoxic Impurities Based on High Performance Chromatography Combined with Mass Spectrometry;** Zheng-Xiang Zhang¹; TAO BO¹; ¹*Agilent Technologies (China), Beijing*
- TP 710 **Rapid Analysis of Histidine, Anserine and Carnosine in Mouse Skeletal Muscle Tissue by HILIC UPLC-MS/MS;** David Hoetker^{1,2}; Adjoa Boakye^{1,2}; Jaron Thomas^{1,2}; Jingjing Zhao^{1,2}; Shahid Baba^{1,2}; ¹*University of Louisville, Louisville, KY*; ²*Diabetes and Obesity Center, U of L, Louisville, KY*
- TP 711 **Determination of Fluticasone Propionate, Salmeterol, Naltrexone, and Buprenorphine in Human Plasma with Ultra-Sensitive LC-MS/MS Methods;** Dawei Zhou¹; Pei Li¹; Thomas moran²; Mohamed Osman¹; Xinping Fang¹; WuXi AppTec, Plainsboro, NJ; ²*Shimadzu Scientific Instruments, Somerset, NJ*
- TP 712 **An Ultrafast LC/MS/MS Method for Characterization and Quantitation of Triton X-100 Extracted from Palm Oil;** Udi Jumhawan¹; Jie Xing¹; Zhaoqi Zhan¹; ¹*Shimadzu Asia Pacific, Singapore, Singapore*
- TP 713 **Quantitation of Endogenous β -Hydroxy- β -Methylbutyric Acid in Human Blood: Comparison between Dried Blood Spot, Dried Plasma Spot, and Liquid Plasma Analysis;** Carl Noren¹; Stefan Ehling¹; Todime Reddy¹; ¹*Abbott Nutrition, Columbus, OH*
- TP 714 **Validated LC-MS/MS Assay for Quantitation of Paclitaxel in Human Seminal Fluid;** Robert Clegg¹; Rachel Sun²; ¹*BASi, West Lafayette, IN*; ²*BASi, West Lafayette, IN*
- TP 715 **Sensitive Quantitative Measurement of Cortisol from Limited Human Hair Samples Using LC-MS/MS;** David W. Erikson¹; Amy V. Kaucher¹; Emily Agan¹; Andrea J. Winchell¹; Steven W. Blue¹; Ashley Scherman²; Cynthia T. McEvoy²; Eliot R. Spindel¹; ¹*Oregon National Primate Research Center, Beaverton, OR*; ²*Oregon Health & Science University, Portland, OR*
- TP 716 **An LC-MS/MS Method to Detect Antibiotic Residues in Distillers Grains to Address Concerns of Potential Antimicrobial Resistance Development;** Hemakanthi De Alwis¹; Kaleb J Dudgeon¹; Upul Nishshanka¹; ¹*Office of Research, Center for Veterinary Medicine, Food and Drug Administration, Laurel, MD*
- TP 717 **A Rugged Bioanalytical Method for Quantification of Liraglutide in Human Plasma by LC-MS-MS;** Karin Keller¹; Heather McLaughlin¹; Laura Binneboese¹; Edward Wells¹; Steve Unger¹; ¹*Worldwide Clinical Trials, Austin, TX*
- TP 718 **Method Development and Validation for the Quantification of Fulvestrant in Human Plasma Using LC-MS/MS;** Guodong Gu¹; Yinghe Li¹; Anna Fiorella¹; Colt Cookson¹; ¹*Alliance Pharma, Malvern, PA*



TUESDAY POSTERS

- TP 719 **Screening Method for Methamphetamine and Amphetamine Using DART® MS Analysis Followed by Chiral Confirmation for D-Methamphetamine;** Craig Aurand¹; Candace Price¹; Sara Smith¹; Emily Barrey¹; ¹MilliporeSigma, Bellefonte, PA
- TP 720 **Analytical Data Longevity and Management for Regulatory Compliance Using AnIML Format and Cloud Technologies;** John Gibbons¹; Viktor N Iassinskii²; Burkhard Schaefer³; ¹SCIEX, Concord, ON; ²Sciex, Concord, ON; ³BSSN Software GmbH, Darmstadt, Germany
- TP 721 **Trimester-Specific Progesterone Reference Intervals Established in Human Serum/Plasma Using a Fast LC-MS/MS Method Coupled with Differential Ion Mobility Spectrometry;** Julie A Ray¹; Joely A Straseski^{1,2}; ¹ARUP Laboratories, Salt Lake City, UT; ²University of Utah, Salt Lake City, UT
- TP 722 **Implementing GMP Impurity Methods on a Single Quadrupole LC/MS;** Laura Hayter¹; Philip Anderson¹; Madelyn Hunsley¹; ¹Avista Pharma Solutions, Longmont, CO
- TP 723 **Chiral Derivatization of D- and L-Flornithine for Enantiomer Identification from a Racemate and Chromatographic Separation;** Abram Brubaker¹; Neal Simmons¹; Ashley Brant¹; Ronald Shoup¹; ¹AIT Bioscience, Indianapolis, IN
- TP 724 **Development of LC-MS/MS Detection Strategies in Rapamycin and Seco-rapamycin Whole Blood Bioanalysis;** Tobias Magers¹; Brian Engel¹; Abram Brubaker¹; Brad King¹; Ashley Brant¹; Ronald Shoup¹; ¹AIT Bioscience, Indianapolis, IN
- TP 725 **A Rugged, Robust, Stereo-Selective LC/MS/MS Method for Simultaneous Determination of Two Enantiomers of a Small Molecule Antibiotic in Human Plasma;** Ze Li¹; Patricia A. Hansen¹; Maral Llewellyn¹; ¹Covance, Indianapolis, IN
- TP 726 **Analysis of Anamorelin Stereoisomers in Human Plasma Using Coupled Achiral / Chiral HPLC with Tandem Mass Spectroscopy Detection;** Steven X. Yan¹; Anika Pippin¹; Yu-Hui Ann Fu¹; Julie Showalter¹; Gene Ray¹; Alberto Bernareggi²; Elizabeth Duus³; Yansheng Liu¹; ¹KCAS Bioanalytical Services, Shawnee, KS; ²Helsinn Healthcare SA, Lugano, Switzerland; ³Helsinn Therapeutics (US), Inc., Iselin, NJ
- TP 727 **A High Sensitivity LC/MS/MS Method for Quantitative Analysis of Five Carcinogenic Dyes in Textiles;** Yin Ling Chew¹; Felicia Xue Qi Tan²; Yi Hao Wee³; Jarren Ling Yao Tuang²; Djohan Kesuma¹; Jie Xing¹; Zhaoqi Zhan¹; ¹Shimadzu Asia Pacific, Singapore; ²School of Physical and Mathematical Science, Nanyang Technical University, Singapore; ³National University of Singapore





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

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AMBIENT IONIZATION: APPLICATIONS II 001 - 034

- WP 001 **Spontaneous Desalting Droplet Spray Ionization for Direct and Sensitive Analysis of Seawater Sample;** Hong Zhang¹; Jing He²; Na Li²; Jie Jiang²; ¹State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin, China; ²School of Marine Science and Technology, Harbin Institute of Technology at Weihai, Weihai, China
- WP 002 **Development of an In Vivo Real-time Monitoring System using Probe Electrospray Ionization/ Tandem Mass Spectrometry (PESI/MS/MS) and its Preliminary Applications;** Kei Zaitzu^{1,2}; Yumi Hayashi¹; ³Tasuku Murata⁴; Tomomi Ohara²; Stéphane Moreau⁵; Maiko Kusano²; Hiroki Nakajima⁶; Hiroshi Tanihata⁴; Hitoshi Tsuchihashi²; Tetsuya Ishikawa³; Akira Ishii²; ¹In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; ²Department of Legal Medicine and Bioethics, Nagoya

- University Graduate School of Medicine, Nagoya, Japan; ³Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; ⁴Shimadzu Corporation, Kyoto, Japan; ⁵Shimadzu Europe GmbH, Duisburg, Germany; ⁶European Innovation Center, Shimadzu Europa GmbH, Duisburg, Germany
- WP 003 **High-throughput Intact Metabolome Analysis of Mouse Biological Specimens by Probe Electrospray Ionization/Tandem Mass Spectrometry (PESI/MS/MS);** Yumi Hayashi^{1,2}; Kei Zaitzu^{1,3}; Tasuku Murata⁴; Shiono Baba³; Tomomi Ohara³; Stéphane Moreau⁵; Maiko Kusano³; Hiroki Nakajima⁶; Hiroshi Tanihata⁴; Hitoshi Tsuchihashi³; Akira Ishii³; Tetsuya Ishikawa²; ¹In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; ²Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; ³Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; ⁴Shimadzu Corporation, Kyoto, Japan; ⁵Shimadzu Europa GmbH, Duisburg, Germany; ⁶European Innovation Center, Shimadzu Europa GmbH, Duisburg, Germany
- WP 004 **Combining Molecularly Imprinted Polymer (MIP) and Paper Spray Mass Spectrometry for Agrochemical Screening in Foodstuffs;** Boniek Gontijo Vaz¹; Igor Pereira¹; Andréia Rodrigues Chaves¹; ¹Federal University of Goiás, Goiânia, GO
- WP 005 **Coupling PaperSpray Technology to High-End Orbitrap Mass Spectrometry;** Kerry Hassell¹; Maria C. Prieto Conaway²; ¹ThermoFisher Scientific, Somerset, NJ; ²ThermoFisher Scientific, San Jose, CA
- WP 006 **Depth-resolved Metabolite Analysis on a Plant Surface by Nanospray Desorption Electrospray Ionization (nano-DESI) Mass Spectrometry;** Sangwon Cha¹; Gyuwoong Jun¹; Dongkun Lee¹; Purum Kim¹; ¹Hankuk University of Foreign Studies, Yongin, South Korea
- WP 007 **Illumination-assisted Droplet Spray Ionization: In Situ Analysis and Real-time Monitoring of Photocatalytic Reactions;** Jie Jiang¹; Hong Zhang²; Na Li¹; ¹School of Marine Science and Technology, Harbin Institute of Technology at Weihai, Weihai, China; ²State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin, China
- WP 008 **Improving Quantification using PaperSpray Ionization Coupled to Ion Trap Mass Spectrometry for Clinical Research;** Cornelia Leonie Boeser¹; Linfan Li¹; Jae C. Schwartz¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 009 **Investigating the Structural Transitions of Proteins during Dissolution by Mass Spectrometry;** Xiaoyun Gong¹; Xingchuan Xiong²; Xiang Fang²; ¹Beijing, Beijing; ²National Institute of Metrology, Beijing, China
- WP 010 **Molecular Discrimination of Follicular Thyroid Adenomas and Carcinomas using Ambient Ionization Mass Spectrometry;** Rachel J. DeHoog¹; Jialing Zhang¹; Elizabeth Alore²; Wendong Yu²; Rob Tibshirani³; Anton F. Engelsman^{4,5}; Stan B. Sidhu^{4,5}; James Suliburk²; Livia S. Eberlin¹; ¹University of Texas at Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX; ³Stanford University, Stanford, California; ⁴Royal North Shore Hospital, Sydney, Australia; ⁵University of Sydney, Sydney, Australia
- WP 011 **Online Examination of Catalytic Oxidation of Glucose by Ambient Liquid-Assisted Ionization Mass Spectrometry;** Yan Wang¹; Jin Ouyang¹; Na Na¹; ¹Beijing Normal University, Beijing, China
- WP 012 **Picomole-Scale Real-Time Photoreaction Screening: Discovery of the Visible-Light-Promoted Dehydrogenation of Tetrahydroquinolines under Ambient Conditions;** Qiongqiong Wan¹; Suming Chen²;



WEDNESDAY POSTERS

- Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH; ²Johns Hopkins University, Baltimore, MD
- WP 013 **Preparative Electrospray and Preparative Reactive Extractive Electrospray for Route Prediction and Optimization of Atropine Synthesis in Microfluidics;** Caitlin Falcone¹; Zinia Jaman¹; Michael Wlekinski¹; Andy Koswara¹; David H. Thompson¹; R. Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- WP 014 **The Utility of Hydrophobic Paper Strips in the Direct Analysis of Dried Biofluids Using Mass Spectrometry;** Deidre E. Damon¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 015 **Thread Spray Mass Spectrometry for In-Situ Analysis of Capsaicinoids;** Sierra Jackson¹; Devin J. Swiner¹; Bridget K. Walsh¹; Yaman Kouatli¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 016 **Whole Body Skin Imaging of Medicines and Metabolites by Thermal Desorption-Electrospray Ionization/Mass Spectrometry;** Jentia Shiea¹; Jia-Ming Lin¹; Yang-Kuang Pan¹; Yu-Hsuan Kuo¹; Hung Su¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan
- WP 017 **Acceleration of Claisen-Schmidt Reaction with Preparative Sonic Spray Ionization;** Zhenwei Wei¹; Michael Wlekinski¹; Caitlin E. Falcone¹; Graham Cooks¹; ¹Purdue University, West Lafayette, IN
- WP 018 **Amino Acids Desalt Protein Samples during DESI-MS Analysis;** Roshan Javanshad¹; Elahe Honarvar¹; Andre R. Venter¹; ¹Western Michigan University, Kalamazoo, MI
- WP 019 **Application of T-probe to MS Metabolomics analysis of live single cells;** Renmeng Liu¹; Yanlin Zhu¹; Ning Pan¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK
- WP 020 **Automated PaperSpray Sample Preparation using a Robotic Autosampler for Clinical Research;** Steven L. Reeber¹; Lucas Luethy²; Cornelia Leonie Boeser¹; John Glazier¹; ¹Thermo Fisher Scientific, San Jose, CA; ²CTC Analytics AG, Zwingen, Switzerland
- WP 021 **Detection and Imaging of Thermochromic Ink Compounds in Erasable Pens using Desorption Electrospray Ionization Mass Spectrometry (DESI-MS);** Amin Khatami¹; Shamina Prova S. Prova¹; Aafreen Bagga¹; Michelle Ting¹; Gurnoor Brar¹; Demian R. Iffa¹; ¹York University, Toronto, ON, Canada
- WP 022 **Distinguishing Non-Small Cell Lung Cancer Subtypes by Desorption Electrospray Ionization Mass Spectrometry;** Alena Bensussan¹; Tanweer Zaidi²; Ruth Katz²; Erik Cressman²; LIVIA S. EBERLIN¹; ¹University of Texas at Austin, Austin, TX; ²MD Anderson Cancer Center, Houston, TX
- WP 023 **Evaluation of Stainless Steel Electrospray Electrodes in Micro LC-MS/MS Analysis;** Tomasz Bienkowski^{1,2}; Konrad Piotr Kowalski^{1,2}; ¹MS Ekspert Sp. z o.o., Gdańsk, Poland; ²Masdiag Sp. z o.o., Warszawa, Mazowieckie
- WP 024 **Metabolite, Lipid, and Peptide Analysis of Single Neurons of Known Function in Lymnaea stagnalis by Capillary Microsampling Mass Spectrometry;** Linwen Zhang¹; Nikkita Khattar¹; Zita Zrinyi²; Zsolt Pirger²; Ildiko Kemenes³; Gyorgy Kemenes³; Akos Vertes¹; ¹The George Washington University, Washington, DC; ²Balaton Limnological Institute, Tihany, Hungary; ³University of Sussex, Brighton, UK
- WP 025 **Methodologies for Investigating Neurodegenerative Disorders using a Liquid-Microjunction Surface Sampling Probe;** Emily L. Gill¹; Megan Marks¹; Richard A. Yost¹; Vinata Vedam-Mai¹; Timothy J. Garrett¹; ¹University of Florida, Gainesville, FL
- WP 026 **Negative Ion Paper Spray for the Detection of Acidic Compounds;** Josiah McKenna¹; Trevor Glaros²; Nicholas E. Manicke¹; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²US Army ECBC, Aberdeen Proving Ground, MD
- WP 027 **Paper Spray High-Resolution Accurate-Mass Spectrometry for Rapid Quantitation of NSAID Drugs in Equine Plasma;** David J. Borts¹; Joseph H. Kennedy²; ¹Iowa State University, Ames, IA; ²Prosolia, Inc., Indianapolis, IN
- WP 028 **Predictive Models of Negative Ion Electrospray Response Explored through Machine Learning Applications;** Melanie T. Odenkirk¹; Ren T. Blackart¹; James M. Matilla¹; Michael L. Poltash¹; Stephen K. Lucas¹; Christine A. Hughey²; Jeff Jones³; ¹James Madison University, Harrisonburg, VA; ²James Madison University, Harrisonburg, VA; ³SoCal Bioinformatics Inc., Glendale, CA
- WP 029 **Rapid Analysis of Forensic Related Samples using Ambient Ionization Techniques Coupled to High Resolution Mass Spectrometers;** Eshwar Jagerdeo¹; Amanda Wriston²; ¹FBI Laboratory, Quantico, VA; ²FBI Laboratory, Huntsville, AL
- WP 030 **Reaction Screening using Accelerated Reactions in Leidenfrost Droplets;** Kiran Iyer¹; H. Samuel Ewan²; Seok-Hee Hyun²; Michael Wlekinski²; David H. Thompson²; R. Graham Cooks²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN
- WP 031 **Direct Analysis of Alloys by Electrochemistry Spray Ionization Mass Spectrometry;** Jiaquan Xu¹; Tengao Zhu¹; Runhan Yan¹; Huanwen Chen¹; ¹East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China
- WP 032 **MS Chemical Fingerprints Reveal the Molecular Dependence of Exhaust Particulate Matters on the Engine Speed;** Yi Li¹; Hua Zhang¹; Kun Liu¹; Feifan Jie¹; Liang Zhu¹; Huanwen Chen¹; ¹East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China
- WP 033 **Rapid Identification of Meat Species by Internal Extractive Electrospray Ionization Mass Spectrometry of Hemoglobin Selectively Extracted on Functionalized Graphene Oxide;** Lili Song¹; Jiaquan Xu¹; Konstantin Chingin¹; Huanwen Chen¹; ¹East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China
- WP 034 **Investigation on the Dehydroxylation of Hydroxyl Polycyclic Aromatic Hydrocarbons by Ambient Mass Spectrometry;** Xiaoping Zhang¹; Yi Li¹; Jiaquan Xu¹; Huanwen Chen¹; ¹East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China
- BIOMARKERS: QUANTITATIVE ANALYSIS II**
035 - 064
- WP 035 **High-thought Determination of Tryptophan and Kynurenine in IDO Assay by LC-MS/MS;** Xinfu Fu¹; Hongmei Wang¹; YI TAO¹; Xinping Fang¹; Xin Zhang¹; ¹WuXi AppTec Co., Shanghai, China
- WP 036 **Development of an LC-MS/MS Method for the Quantitation of Fatty Acid Dicarboxylates, Potential Biomarkers for OATP Function;** Weiqi Chen¹; Hong Shen²; Yurong Lai²; William Humphreys²; Jinping Gan²; ¹Bristol-Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb, Princeton, NJ
- WP 037 **Determination of a Double-stranded Small Interfering RNA and its Two Single Strands in Sprague-Dawley Rat Plasma by LC-MS/MS;** Yanfu Ren¹; Lili Xing¹; YI TAO¹; Xinping Fang¹; Xin Zhang¹; ¹WuXi AppTec Co., Shanghai, China
- WP 038 **Differentiating Modes of Drug Induced Liver Injury using Parallel Reaction Monitoring LC-MS;** Michelle R. Robinson¹; Lei Guo²; Raymond J. Gonzalez¹; Kara M. Pearson¹; Kevin P. Bateman¹; Daniel S. Spellman¹; ¹Merck Research Laboratories, West Point, PA; ²Sanofi Genzyme, Cambridge, MA



- WP 039 **Sensitive and Specific Determination of N-Linked Oligomannosides in Mouse Plasma and Brain Tissue Using LC-HRAM Method**; Yuhuan Ji¹; Qian Li¹; Jian Shi¹; John Chen¹; Chengjie Ji¹; Laixin Wang¹; Mo Qatanani²; Meng Chen²; ¹NovaBioAssays LLC, Woburn, Massachusetts; ²Alexion Pharmaceuticals, Lexington, Afghanistan
- WP 040 **Absolute Quantitation of Acetaminophen-Modified HSA by LC-MRM**; Timon Geib¹; André LeBlanc¹; Tze Chieh Shiao¹; Ghazaleh Moghaddam¹; Amal Guesmi¹; René Roy¹; Lekha Sleno¹; ¹UQAM, Montreal, QC, Canada, Canada
- WP 041 **SWATH Proteome Phenotyping of Melanoma Identifies Biomarkers of MEK Response and Post Biopsy Survival**; Christoph Krisp¹; Robert Parker²; Dana Pascovici¹; James Wilmott³; John F Thompson³; Graham J Mann³; Nicholas Hayward⁴; Richard A Scolyer³; Mark P Molloy¹; ¹Australian Proteome Analysis Facility, Sydney, NSW; ²Imperial College, London, UK; ³Melanoma Institute Australia, Sydney, Australia; ⁴Oncogenomics Laboratory, QIMR Berghofer Medical Research Institute, Brisbane, Australia
- WP 042 **Phosphoproteins in Extracellular Vesicles as the Candidate Markers for Breast Cancer**; I-Hsuan Chen¹; Liang Xue¹; Chuan-Chih Hsu¹; Juan Sebastian Paez Paez¹; Li Pan¹; Hillary Andaluz Aguilar¹; Michael K Wendt¹; Anton Iliuk¹; Jian-Kang Zhu¹; Andy Tao¹; ¹Purdue University, West Lafayette, IN
- WP 043 **Biomonitoring Cooked Meat Carcinogen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in Human Hair and Prostate by Nano Liquid Chromatography-High Resolution Tandem Mass Spectrometry**; Shun Xiao^{1,2}; Jingshu Guo^{1,2}; Byeong Hwa Yun^{1,2}; Peter W. Villalta¹; Suprita Krishna³; Resha Tejapaul³; Paari Murugan⁴; Christopher J. Weight³; Robert J. Turesky^{1,2}; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN; ³Department of Urology, University of Minnesota, Minneapolis, MN; ⁴Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN
- WP 044 **Proteomic Signature of BRCA1-like Triple-Negative Breast Cancers with Homologous Recombination Deficiency**; Youdinghuan Chen^{1,2}; Nicole P. Jenkins¹; Yue Wang³; Johnathan D. Marotti⁴; Chao Cheng^{3,5,6}; Lucas A. Salas²; Brock C. Christensen^{2,3,6}; Todd W. Miller^{3,6}; Arminja N. Kettenbach^{1,6}; ¹Department of Biochemistry and Cell Biology, Dartmouth College, Lebanon, NH; ²Department of Epidemiology, Dartmouth College, Lebanon, NH; ³Department of Molecular and Systems Biology, Dartmouth College, Lebanon, NH; ⁴Department of Pathology and Laboratory Medicine, Dartmouth College, Lebanon, NH; ⁵Department of Biomedical Data Science, Dartmouth College, Lebanon, NH; ⁶Norris Cotton Cancer Center, Lebanon, NH
- WP 045 **Development of Chemical Isotope Labeling LC-MS for Metabolite Biomarker Discovery of Alzheimer's Disease in a Mouse Model**; Xiaohang Wang¹; Xinyun Gu¹; Wei Han¹; Jing Yang¹; David Westaway¹; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada
- WP 046 **High Sensitivity CZE-ESI-MS Investigations and Applications in Proteomics**; Emily Amenson¹; Liangliang Sun²; Norman J Dovichi¹; ¹University of Notre Dame, Notre Dame, IN; ²Michigan State University, Lansing, MI
- WP 047 **Novel GC-MS Method for the Characterization and Quantification of Short Chain Fatty Acids, Malonaldehyde, and Muconic Acid in Biological Samples**; Blake Lynch¹; Daniel Conklin¹; Aruni Bhatnagar¹; Sanjay Srivastava¹; Pawel Lorkiewicz²; ¹University of Louisville, Louisville, KY; ²University of Louisville, Louisville, KY
- WP 048 **Targeted Proteomic Characterization of Human Multipotent Stromal Cells Therapeutic Properties**; Miljan Kuljanin¹; David A. Hess^{2,3}; Gilles A. Lajoie¹; ¹Don Rix Protein Identification Facility, Department of Biochemistry, Schulich School of Medicine and Dentistry, University of Western Ontario, London, Ontario; ²Kremlb Centre for Stem Cell Biology, Molecular Medicine Research Group, Robarts Research Institute, London, Ontario; ³Department of Physiology and Pharmacology, Schulich School of Medicine and Dentistry, University of Western Ontario, London, Ontario
- WP 049 **Intelligent Algorithm using Particle Swarm Optimization (SWARM) with Enhanced Limit of Detection for Large Molecule Applications**; Huy Bui¹; Christian Klein²; Alex Zhu³; Alex Mordehai²; Gregor Overney²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Santa Clara, CA; ³Agilent Technologies, Inc., Wilmington, DE
- WP 050 **High-precision Quantification of Warburg Effect Enzymes in a Comprehensive Panel of Breast Cancer Patient Derived Xenografts**; Robert W. Sprung¹; Petra Erdmann-Gilmore¹; Sherri R. Davies¹; John A. Wrobel²; Rose Connors¹; Yiling Mi¹; Lisa J. Zimmerman³; Daniel C. Liebler³; Reid Townsend¹; ¹WUSTL, St. Louis, MO; ²UNC - Chapel Hill, Chapel Hill, NC; ³Vanderbilt University Medical Center, Nashville, TN
- WP 051 **Clinical Tracers: A Simple, Rapid and Simultaneous LC-MS Method to Measure Stable Isotope Enrichment of Glucose, Glycerol And Palmitic Acid**; Peter J. Walter¹; H. Martin Garraffo¹; Stephanie Chung¹; Rebecca J Brown¹; ¹NIH, Bethesda, MD
- WP 052 **A Generic Kit-Based Approach for LC-MS/MS Quantification of Urinary Albumin for Clinical Research**; Mary E. Lame¹; Caitlin M. Dunning²; Paula M. Orens²; ¹Waters Technologies Corporation, Milford, MA; ²Waters Corporation, Milford, MA
- WP 053 **LC-MS/MS Quantification of Urine Glycosaminoglycans in Children with Severe Malaria**; Haoyue Zhang¹; J. Brice Weinberg²; Nicholas M. Anstey³; Matthew P. Rubach²; Tsin W. Yeo⁴; Salvatore Florence⁵; Esther D. Mwaikambo⁵; Donald L. Granger⁶; David S. Millington¹; ¹Duke University Pediatrics, Durham, NC; ²Duke University and VA Medical Centers, Durham, NC; ³Menzies School for Health Research and Charles Darwin University, Darwin, Australia; ⁴Lee Kong Chian School of Medicine, Nanyang Technological University, Nanyang, Singapore; ⁵Hubert Kairuki Memorial University, Dar es Salaam, Tanzania; ⁶University of Utah School of Medicine and VA Medical Center, Salt Lake City, UT
- WP 054 **LC-SRM to Quantify Suitable Tau Peptides to Evaluate Animal Model and Follow Disease Progression**; Chloe Bardet¹; Tanguy Fortin¹; Rodolphe Billiras²; Arnaud François²; Valérie Pasteau²; Karine Albinet²; Gaëlle Rollin-jego²; Fabrice Iop²; Alain Gobert²; ¹Anaquant, Villeurbanne, France; ²Neuropsychiatry Innovation Therapeutic Pole, Institut de Recherches Servier, Croissy sur Seine, France
- WP 055 **MRM-based Validation Assay for Serum Proteomic Alterations in Meningioma Patients**; Shuvolina Mukherjee¹; Sujata Wajunji¹; Purushottam Sutar²; Ajit Datar²; Aliasgar Moiyadi³; Epari Sridhar³; Sanjeeva Srivastava¹; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ³Tata Memorial Hospital, Parel, Mumbai, India
- WP 056 **Quantitation of Orotic Acid in Human Urine on the AB SCIEX API-4000 LC-MS/MS System**; YONG-XI LI¹; Joshua Froning¹; Guangchun Zhou¹; ¹Medpace Bioanalytical Laboratory, Cincinnati, OH
- WP 057 **Multi-Matrix LC-MS/MS Methods for Quantification of Neurological Biomarkers N-Acetyl Aspartic Acid and Homocarnosine**; Dewakar Sangaraju¹; Xiao Ding¹; Sheerin K. Shahidi-Latham¹; ¹Genentech, Inc., South San Francisco, CA



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- WP 058 **A Rapid Measurement of Urinary 6-Sulfatoxymelatonin (aMT6s) as a Biomarker Using HPLC-Tandem Mass Spectrometry;** Tian-Sheng Lu¹; Guandong Zhang¹; Feng Yin¹; Joshua Froning¹; Emily Epure¹; Yong-Xi Li¹; ¹*Medpace Bioanalytical Laboratory, Cincinnati, OH*
- WP 059 **Quantitative HPLC-MS/MS Analysis of Human Apolipoproteins Utilizing SILuMab as a Commercially Available Internal Standard and Standard 96-Well Plates;** Caleb Robinson¹; Ann Hoffman¹; Chad D. Christianson¹; Jennifer S.D. Zimmer¹; Shane R. Needham¹; ¹*Alturas Analytics, Inc., Moscow, ID*
- WP 060 **An LC-MS/MS Measurement of Cortisol as a Biomarker in Human Urine;** Feng Yin¹; Andrew Swenson¹; Emily Epure¹; Tian-Sheng Lu¹; Yong-Xi Li¹; ¹*Medpace Inc., Cincinnati, OH*
- WP 061 **Direct Measurement of Serotonin Synthesis as a Predictive Marker of Serotonin Pharmacodynamics and Disease-Induced Dysregulation;** Richard Welford¹; Magali Vercauteren¹; Annette Trébaul¹; Christophe Cattaneo¹; Doriane Eckert¹; Marco Garzotti¹; Patrick Sieber¹; Jérôme Segrestaa¹; Rolf Studer¹; Peter M Groenen¹; Oliver Naylor¹; ¹*Actelion Pharmaceuticals, Allschwil*
- WP 062 **Analysis of Deuterated Phenanthrene Metabolites in Human Urine by GC-NICI-MS/MS-SRM;** Kai Luo¹; Viviana Paiano¹; Steven G. Carmella¹; Jon B. Hochalter¹; Naomi Fujioka¹; Stephen S. Hecht¹; ¹*University of Minnesota, Minneapolis, MN*
- WP 063 **Simultaneous Quantitative Determination of Synthetic Cathinones Enantiomers in Urine and Plasma using GC-NCI-MS;** Rashed Alrumaithi¹; Mohammad Almeetani²; Anas Alaidaros²; Adnan Lanjawi¹; Khaled Alsumaiti¹; ¹*Dubai Police, Dubai, Dubai; 2United Arab Emirates University, Al Ain, United Arab Emirates*
- WP 064 **Calculating Biological Age Using Label-Free Mass Spectrometry Based Proteomics;** Harris Bell-Temin¹; Matthew Yousefzadeh²; Jessica Snyder³; Warren Ladiges³; Paul Robbins²; Laura Niedernhofer²; Nathan A Yates¹; ¹*University of Pittsburgh School of Medicine, Pittsburgh, PA; 2The Scripps Research Institute, Jupiter, FL; 3University of Washington, Seattle, WA*

DATA-INDEPENDENT ACQUISITION 065 - 088

- WP 065 **Profiling Biochemical Individuality: Human Personal Omics Profiling (hPOP);** Sara Ahadi¹; Hannes Roest¹; Liang Liang¹; Christie Hunter²; Mike Snyder¹; ¹*Stanford School of Medicine, Stanford, CA; 2SCIEX, Redwood City, CA*
- WP 066 **Characterization of Data-Independent Acquisition (DIA) Capabilities of a Q-TOF Instrument for Complex Proteomics Samples;** Stephanie Kaspar-Schoenefeld¹; Thomas Kosinski¹; Romano Hebel¹; Pierre-Olivier Schmit¹; Gary Kruppa¹; ¹*Bruker Daltonik GmbH, Bremen, Germany*
- WP 067 **PepShare Mapper – A Strategy to use Shared Peptides from SWATH-MS to Quantitate Isoforms and Analyze Mixed Species Proteomes;** Christoph Krisp¹; Jemma Wu¹; Mark P. Molloy¹; ¹*Australian Proteome Analysis Facility, Sydney, NSW*
- WP 068 **Analysis of m/z Distribution of Tryptic Peptides in Various Types Biological Samples, Supporting Generic DIA Strategies;** Faraz Rashid¹; Manoj Pillai¹; Dipankar Malakar¹; ¹*AB SCIEX, Gurugram, Haryana*
- WP 069 **Quantitative Analysis of Proteomic Samples using a Novel Scanning Quadrupole Method;** Sarah Lennon¹; Gushinder Kaur-Atwal¹; Erika P Parkinson²; Paul J. Skipp²; Thérèse McKenna¹; ¹*Waters Corporation, Wilmslow; 2Centre for Biological Sciences, University of Southampton, Southampton, UK*
- WP 070 **Future Directions for Data-Independent Acquisition Modes Utilising a Scanning Quadrupole on Q-ToF Instruments;** Keith G. Richardson¹; Jason L. Wildgoose¹; Chris Hughes¹; Praveen Harapanahalli¹; ¹*Waters Corporation, Wilmslow, UK*
- WP 071 **Enhancing the Throughput and Robustness of DIA using a 150 µm EASY-Spray Column;** Joshua Nicklay¹; Kerry M Hassell¹; Aran Paulus²; ¹*Thermo Fisher Scientific, Somerset, NJ; 2Thermo Fisher Scientific, San Jose, CA*
- WP 072 **Utilization of IM-MS Deconvolution for Reduced LC Separation Time Requirements in High-throughput Proteomics;** Michael E. Pettit¹; Matthew R. Brantley¹; Fabrizio Donnarumma²; Kermit K. Murray²; Touradj Solouki¹; ¹*Baylor University, Waco, TX; 2Louisiana State University, Baton Rouge, LA*
- WP 073 **Building a Community Platform for High-Throughput Data Independent Acquisition Analysis on the Cloud;** Jarrett Egerton¹; Brian Searle^{1,2}; Sonia Ting¹; Lindsay K Pino¹; Han-Yin Yang¹; Austin Keller¹; Vagisha Sharma¹; Brendan MacLean¹; Michael J MacCoss¹; ¹*University of Washington, Seattle, WA; 2Proteome Software, Portland, OR*
- WP 074 **A New Approach to Generate High Quality Spectral Libraries and Determine Signal Interference in DIA Experiments;** Antoine Lesur¹; Petr V. Nazarov¹; Sang Yoon Kim¹; Sébastien Gallien²; Gunnar Dittmar¹; Daniel Ayoub¹; ¹*Proteome and Genome Research Unit, Department of Oncology, Luxembourg Institute of Health, Strassen, Luxembourg; 2Thermo Fisher Scientific, Courtaboeuf, France*
- WP 075 **Data Independent Acquisition with a Fast Scanning, Low Resolution Hybrid Quadrupole-Linear Ion Trap;** Austin Keller¹; Jarrett Egerton¹; Brian Searle^{1,2}; Lindsay K Pino¹; Philip M Remes³; Romain Huguet³; Michael J MacCoss¹; ¹*University of Washington, Seattle, WA; 2Proteome Software, Portland, OR; 3Thermo Fisher Scientific, San Jose, CA*
- WP 076 **Using Orbitrap's Unique Strengths, Combined with DeepDIA's DeepSearch Protocol, to Maximize Sensitivity on DIA-capable Orbitrap Instruments;** Dennis Goldfarb¹; Gautam Saxena¹; ¹*DeepDIA, Bethesda, MD*
- WP 077 **A Dual Workflow to Improve the Protein Coverage for Plasma Data-Independent Analysis;** Shenyang Zhang¹; Qin Fu¹; Vidya Venkatraman¹; Ronald Holewinski¹; Jennifer Van Eyk¹; ¹*Cedars-Sinai Medical Center, Los Angeles, CA*
- WP 078 **GPGPU-based Database-Search Engine for Feature Identification with DIA data;** Yu Gao¹; John R. Yates III¹; ¹*The Scripps Research Institute, La Jolla, CA*
- WP 079 **Structural Elucidation of an Unknown Compound in Avocado Fatty Acid Methyl Esters (FAMES) Extract Using APGC-HRMS;** Lauren Mullin^{1,2}; Dana Krueger³; Melissa Phillips⁴; Sarah Dowd⁵; Joe Romano¹; Kenneth Rosnack¹; ¹*Waters Corporation, Milford, MA; 2Örebro University, Örebro, Sweden; 3Krueger Food Laboratories Inc, Chelmsford, MA; 4NIST, Gaithersburg, MD; 5Waters Corporation, Beverly, MA*
- WP 080 **Having a Free Lunch: A Combined DIA+DDA Approach Towards Spectral Library Generation for DIA Analysis using Spectronaut;** Tejas Gandhi¹; Lynn Verbeke¹; Oliver M. Bernhardt¹; Roland Bruderer¹; Jan Muntel¹; Lukas Reiter¹; ¹*Biognosys, Schlieren, Zurich*
- WP 081 **Deep Proteomic Profiling using Data Independent Acquisition;** Reta Birhanu Kitata^{1,2,3}; Pei-Yi Lin¹; Ching-Tai Chen⁴; Chia-Feng Tsai⁵; Alexey I. Nesvizhskii⁶; Ting-Yi Sung⁴; Yu-Ju Chen¹; ¹*Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; 2Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan; 3Molecular Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei City, Taiwan; 4Institute of Information Science, Academia Sinica, Taipei City, Taiwan; 5Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; 6Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, MI*



- WP 082 **Data Independent Acquisition of Small Molecules by Resonance Collision Induced Dissociation;** Philip M. Remes¹; Austin Keller²; Jarrett Egerton²; Richard Johnson²; Romain Huguet¹; Michael J MacCoss²; Jae C. Schwartz¹; ¹Thermo Fisher Scientific, San Jose, California; ²University of Washington, Department of Genome Sciences, Seattle, WA
- WP 083 **From Targeted to Untargeted DNA Damage Screening — DNA Adduct “Omics” Analysis by High Resolution Multi-stage Mass Spectrometry;** Jingshu Guo^{1,2}; Peter W. Villalta¹; Robert J. Turesky^{1,2}; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN
- WP 084 **Optimization of SONAR Elevated Energy Ramps Applied to Different Molecule Classes;** Chris Hughes¹; Lee A Gethings¹; Jonathan P Williams¹; Johannes P.C. Vissers¹; James I Langridge¹; ¹Waters, Manchester, UK
- WP 085 **Comprehensive DIA on a Q-ToF Instrument for Discovery and Quantitative Analysis Utilising a Scanning Quadrupole;** Jason Wildgoose¹; Keith Richardson¹; Martin R. Green¹; ¹Waters Corporation, Wilmslow, UK
- WP 086 **De novo DIA Analysis (DDA);** Richard S. Johnson¹; Brian Searle²; Austin Keller²; Michael J MacCoss²; ¹, Mercer Island, WA; ²University of Washington Genome Sciences, Seattle, WA
- WP 087 **Universal Data-Independent LC-MS/MS Workflow for Host Cell Protein Characterization and Quantification in Biopharmaceutical Product Purification Process;** Lei Xiong¹; Yihan Li¹; Stephen Tate²; Todd Stawicki³; Edita Bottonic-Sehic⁴; Mark Schofield⁴; Vincent Ravault⁵; Sean McCarthy³; Hua-Fen Liu¹; ¹SCIEX, Redwood City, CA; ²SCIEX, Concord, ON, Canada; ³SCIEX, Framingham, MA; ⁴Pall Corporation, Westborough, MA; ⁵Pall Corporation, Cergy, France
- WP 088 **Two-Dimensional Mass Spectrometry in a Linear Ion Trap;** Maria A. van Agthoven¹; Christopher A. Wootton¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, Midlands, UK
- DRUG METABOLISM: QUALITATIVE AND HIGH THROUGHPUT ANALYSIS**
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- WP 089 **Bitransformation and Metabolic Profile of the Roots of the Polygala with Intestinal Microflora In Vitro by UPLC-MS Method;** Zhiqiang Liu¹; Guifang Feng²; Shu Liu¹; ¹National Center for Mass Spectrometry in Changchun & Key Laboratory for Traditional Chinese Medicine Chemistry and Mass Spectrometry of Jilin province & Chemical Biology Laboratory, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China; ²University of Science and Technology of China, Hefei, China
- WP 090 **In vitro Investigation of Metabolic Profiling of Newly Developed Topoisomerase Inhibitors (Ethyl Fluorescein Hydrazones, EtFLHs) in RLMS by LC-MS/MS;** Adnan A Kadi¹; Nasser S Al-Shakli¹; A. F. M. Motiur Rahman¹; ¹King Saud University, Riyadh, Riyadh
- WP 091 **A Rapid and Sensitive LC-HRMS Method for Detection of Glutathione-Trapped Reactive Metabolites using a High-Resolution Orbitrap System;** Zhicun Wang¹; Ying Fang¹; Dan Rock¹; Ji Ma¹; ¹Amgen, South San Francisco, CA
- WP 092 **Simultaneous Determination of Metabolic Stability and Metabolite Identification using a High-Resolution Mass Spectrometry;** Zhicun Wang¹; Min Jiang¹; Chi-Chi Peng¹; Dan Rock¹; Ji Ma¹; ¹Amgen, South San Francisco, CA
- WP 093 **Strain and Sex Differences in Metabolism in Rats: Assessment of Buspirone Metabolism by High Resolution LC/MS Analysis;** Rutali R. Brahme¹; Jennifer L. Dumouchel¹; Upendra A. Argikar¹; ¹Novartis Institutes for BioMedical Research, Cambridge, MA
- WP 094 **Profiling of In Vitro and In Vivo Metabolites of Novel TKIs using LC-MS/MS Method: Metabolic Stability and Bioactivation Pathway Elucidation;** Adnan A. Kadi¹; Hany W. Darwish^{1,2}; Mohamed W Attwa^{1,2}; Sawsan M. Amer²; ¹College of Pharmacy, King Saud University, Riyadh, Saudi Arabia; ²Faculty of Pharmacy, Cairo University, Cairo, Egypt
- WP 095 **A New Method for Analyzing MSE/All Ions Fragmentation in Xenobiotic Metabolism Studies;** Richard Lee¹; Vitaly Lashin²; Alexandre Sakarov²; Andrey Paramonov²; ¹ACD/Labs, Burlington, ON, Canada; ²ACD/Labs, Moscow, Russia
- WP 096 **A New Biotransformation Prediction Engine Integrated into a Metabolite Identification Solution;** Richard Lee¹; Rytis Kubilius²; Vitaly Lashin³; Alexandre Sakarov³; Andrey Paramonov³; ¹ACD/Labs, Burlington, ON, Canada; ²ACD/Labs, Vilnius, Lithuania; ³ACD/Labs, Moscow, Russia
- WP 097 **Revisit Metabolism and Bioactivation of Ketoconazole using LC-MS-Based Metabolomics;** Ju-Hyun Kim¹; Won-Gu Choi¹; Hye Suk Lee¹; ¹College of Pharmacy, The Catholic University of Korea, Bucheon-si, South Korea
- WP 098 **Use of HILIC Chromatography for the Identification of Metabolites of Polar Drugs by HPLC-MS/MS;** Joshua L. Johnson¹; Adam Amaral¹; Jiansheng Haung¹; Ying Liu¹; Mohammad Shadid¹; Amin Kamel¹; ¹Biogen, Cambridge, MA
- WP 099 **Novel Software Algorithm iMassFrag to Automate Drug Metabolite Identification and Mass Spectral Interpretation;** Siwei Li¹; Jing Lu¹; Duxin Sun¹; ¹University of Michigan, Ann Arbor, MI
- WP 100 **Fast and Comprehensive Detection and Characterization of Cyclic Peptide Metabolites using Software-Aided Data Processing Tools;** Ming Yao¹; Eva Duchoslav²; Li Ma¹; Silvi Chacko¹; Mingshe Zhu¹; ¹Bristol-Myers Squibb, Princeton, New Jersey; ²SCIEX, Concord, ON, Canada
- WP 101 **Dipyridamole High Throughput Analysis of Drug Metabolism Cells Assay using LDTD-MS/MS;** Jean Lacoursiere¹; Serge Auger¹; Pierre Picard¹; ¹Phytronix Technologies, Québec, QC, Canada, Canada
- WP 102 **Application of iMassFrag, a Novel Mass Spectral Interpretation Algorithm, to Structural Elucidation of Oxidative Drug Metabolites;** Silvi Chacko¹; Siwei Li²; Xiaoliang Zhuo¹; Weiping Zhao¹; Duxin Sun²; Mingshe Zhu¹; ¹Bristol-Myers Squibb, Princeton, New Jersey; ²University of Michigan, Ann Arbor, MI
- WP 103 **Development of a Sensitive and Selective High Resolution Accurate Mass LC-SIM for the Detection of Oligonucleotides in Biological Matrices;** Heng-Keang Lim¹; Jie Chen¹; Salter Rhys¹; ¹Janssen Pharmaceuticals R&D, Spring House, PA
- WP 104 **A Metabolite ID Workflow on a Small Footprint Benchtop Q-TOF Mass Spectrometer with Automated Software Structure Generation;** Shaokun Pang¹; Ian Moore²; ¹SCIEX, Redwood City, CA; ²SCIEX, Concord, ON, Canada
- WP 105 **Label Free High Throughput Screening of Amino Acid Based Assays: Old Tricks, New Speed using LDTD-MS/MS;** Pierre Picard¹; Sylvain Letarte¹; Serge Auger¹; Jean Lacoursiere¹; ¹Phytronix Technologies, Inc., Quebec, QC, Canada
- WP 106 **High-Throughput and Automated Software Workflow Strategies for Small Molecule Identification and Characterization Using a High Resolution Q-TOF Mass Spectrometer;** Alina Dindyal-Popescu¹; Iris Shek¹; Mohammed Jooyandeh¹; Ian Moore¹; Eva Duchoslav¹; ¹SCIEX, Concord, ON, Canada
- WP 107 **The Application of Research Grade MetabolitePilot™ Software for the Determination of Exenatide Catabolites using HRAM with SWATH Acquisition;** Jeff Plomley¹



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Yi Zhang²; Eva Duchoslav³; DANIEL Villeneuve¹; Kevork Mekhssian¹; Anahita Keyhani¹; *Algorithm Pharma an Altasciences company, Laval, QC, Canada*; ²Sciex, Frammingham, MA; ³Sciex, Concord, ON, Canada

- WP 108 **Horses For Courses – A Comparison of SONAR and Other Data-Independent Acquisition Strategies for Drug Metabolism and Pharmacokinetics**; Russell Mortishire-Smith¹; Jayne Kirk¹; Mark Wrona²; Sherri Naughton²; Kirsten Craven¹; *¹Waters Corporation, Wilmslow, UK; ²Waters Corp, Milford, MA*

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- WP 109 **Toxic Metal Accumulation and Speciation of Foodstuffs in Aquaponics Systems using HPLC and ICP-MS**; Skyler Smith¹; Megan Schmale¹; Julio A. Landero Figuero¹; *¹University of Cincinnati, Cincinnati, OH*
- WP 110 **Quantitative Determination of Heavy Metals in Ayurvedic Tablets using ICPMS**; Ankush Bhone¹; Sampada Khopkar¹; Mangesh Pawar¹; Amol Shinde¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; *¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- WP 111 **Quantitative Determination of Heavy Metals in Whole Blood using Inductively-Coupled-Plasma-Mass Spectrometry (ICPMS) by Microwave Digestion and Dilution Technique**; Sampada Khopkar¹; Mangesh Pawar¹; Amol Shinde¹; Ankush Bhone¹; Ajit Datar¹; Jitendra Kelkar¹; Pratap Rasam¹; *¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- WP 112 **Exposure and Safety Studies of Herbal Supplements from the United States and Nigeria by Inductively Coupled Plasma Mass Spectrometry (ICPMS)**; Olujide Akinbo¹; Kyle Colston¹; *¹Butler University, Indianapolis, IN*
- WP 113 **Evaluating Heavy-Metal Induced Stress in Aquaponics Systems through Phytochelatin**; Megan Schmale¹; Julio A. Landero Figuero²; *¹University of Cincinnati, Cincinnati, OH; ²University of Cincinnati, Cincinnati, OH*
- WP 114 **Elemental Profiling to Combat Illegal Wildlife Trade**; Simin D. Maleknia¹; Keith Leggett²; Chris Marjo²; Mike Letnic²; *¹University of New South Wales, Sydney, NSW; ²University of New South Wales, Sydney, Australia*
- WP 115 **Inductively Coupled Plasma-Mass Spectrometry Coupled with Solid Phase Microextraction for Simultaneous Determination of Heavy Metals in Natural Water**; Ahmad Rohanifar¹; Lidia B. Rodriguez¹; Amila M. Devasurendra¹; Niloofar Alipourasiabi¹; Jon R. Kirchhoff¹; *¹University of Toledo, Toledo, OH*

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- WP 116 **Phosphoproteomic Approach for Deciphering Signaling Pathways in Chlamydomonas Reinhardtii**; Emily G. Werth¹; Evan W. McConnell¹; Inmaculada Concepcion Couso Lianez²; James G. Umen²; Leslie M Hicks¹; *¹UNC Chapel Hill, Chapel Hill, NC; ²Donald Danforth Plant Science Center, St. Louis, MO*
- WP 117 **Thin-Film vs Powder Lignin Pyrolysis Analyzed by Py-GC-dAPCI-TOFMS with In-Source CID**; Evan Larson¹; Carolyn Hutchinson¹; Young-Jin Lee¹; *¹Iowa State University, Ames, IA*
- WP 118 **Lipid Characterization in Genetically Engineered Yarrowia lipolytica by Desorption Electrospray Ionization Mass Spectrometry**; John Lin¹; Lauren T. Cordova²; Hal S. Alper²; Livia S. Eberlin¹; *¹Department of Chemistry, The University of Texas at Austin, Austin, TX; ²McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX*
- WP 119 **Real-Time Monitoring of Single Particle Herbaceous and Woody Biomass in μ Py-dAPCI-TOF MS**; Carolyn Hutchinson¹; Evan Larson¹; Young Jin Lee¹; *¹Iowa State University, Ames, IA*

- WP 120 **The Investigation of the Bio-Oil Produced by Hydrothermal Liquefaction of Different Microalgae Strains using Fourier Transform Mass-Spectrometry and Hydrogen/Deuterium Exchange**; Gleb Vladimirov^{1,2,3,4,5}; Yury Kostyukovich^{1,2,3,4,5}; Igor Popov^{2,3}; Mikhail Vlaskin⁵; Nadezhda Chernova⁶; Sophia Kiseleva⁶; Eugene Nikolaev^{1,2,3}; *¹Skolkovo Institute of Science and Technology, Skolkovo, Russia; ²Institute of Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia; ³Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; ⁴Institute of Biochemical Physics Russian Academy of Sciences, Moscow, Russia; ⁵Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia; ⁶M.V. Lomonosov Moscow State University, Moscow, Russia*
- WP 121 **Characterizing the Range and Specificity of Substrate-Specific Extracellular Enzymes in Caldicellulosiruptor Bescii**; Suresh Poudel^{1,2}; Richard J Giannone²; Mirko Basen³; Farris Poole³; Robert Kelly⁴; Michael W Adams³; Robert L Hettich⁵; *¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Lab, Oak Ridge, TN; ³University of Georgia, Athens, GA; ⁴North Carolina State University, Raleigh, NC; ⁵Oak Ridge National Laboratory, Oak Ridge, TN*
- WP 122 **Experimental Study of the Combustion Kinetics of the Monoterpenes α -Pinene, β -Pinene, and Myrcene in Flames by Photoionization Time-of-Flight Mass Spectrometry**; Thomas Bierkandt¹; Tina Kasper¹; *¹University of Duisburg-Essen, Duisburg, Germany*
- WP 123 **Study of Douglas and Miscanthus Wood Material and Miscanthus Biochar by LDI FT-ICR MS**; Frédéric Aubriet¹; Thierry Ghislain²; Vincent Carré¹; Yann Le Brech²; Ghislain Mauviel²; Anthony Dufour²; *¹Université de Lorraine - LCP-A2MC, Metz, France; ²Université de Lorraine, LRGP, Nancy, France*
- WP 124 **A Multi-Omic Approach to Decipher the Regulatory Mechanisms Controlling Lipid Production in Oleaginous Yeast for the Enhanced Production of Biofuels**; Richard J. Giannone¹; Nancy L. Engle¹; Robert L. Hettich¹; Daniel A. Jacobson¹; Timothy J. Tschaplinski¹; Daniel M. Close¹; *¹Oak Ridge National Laboratory, Oak Ridge, TN*
- WP 125 **Diagnostic Tools for Measuring Early Chemical Signatures of Algae Pond Crash**; Curtis Mowry¹; Matthew W. Moorman¹; Adam S. Pimentel¹; Jerilyn A. Timlin¹; Todd W. Lane²; Carolyn L. Fisher²; Stephen M. Anthony¹; Komandoor Achyuthan²; *¹Sandia National Laboratories, Albuquerque, NM; ²Sandia National Laboratories, Livermore, CA*
- WP 126 **Comparison of Product Distributions from Fast Pyrolysis of Genetic Variants of Poplar by Using a Pyroprobe Inside an APCI Source**; Lan Xu¹; *¹Purdue University, West Lafayette, IN*

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- WP 127 **Targeted and Non-Targeted Metabolomics to Study Developmental Neurotoxicity of Biocides - Metabolomic Pathway Analysis Reveals Developmental Neurotoxic Effects of Pesticides**; Pim Leonards¹; Aiko Barsch²; Magdalene Reinkensmeier²; Andrew Baca³; Heiko Neuweget²; *¹Environment & Health, VU University of Amsterdam, Amsterdam, Netherlands; ²Bruker Daltonics, Bremen, Germany; ³Bruker Daltonics, Fremont, CA*
- WP 128 **Monitoring of human urinary metabolites of biogenic volatile organic compounds using UPLC-MS/MS**; Zhengzhi Xie¹; Pawel Lorkiewicz¹; Ray Yeager II¹; Rachel Keith¹; Sanjay Srivastava¹; Aruni Bhatnagar¹; *¹University of Louisville, Louisville, KY*
- WP 129 **Meet Stringent Detection Requirements for All 13 4-Nonylphenol Isomers in Water using GCMS-SIM**



- and a High Efficiency Ion Source; Katsura Sekiguchi¹; Kamila Kalachova²; Melissa Churley³; Harry Prest⁴; ¹Agilent Technologies Japan, Ltd., Hachioji Site, Japan; ²Agilent Technologies Sales & Services GmbH & Co. KG, Waldbronn, Germany; ³Agilent Technologies, Inc., Santa Clara, CA; ⁴Agilent Technologies Inc., Santa Clara, CA
- WP 130 **Quantification of Persistent Organic Pollutants in Human Blood Using Stir Bar Sorptive Extraction-GC triple Quad-Isotope Dilution Mass Spectrometry**; Weier Hao¹; Anthony Macherone²; H. M. Skip Kingston¹; Edward Pfannkoch³; Matt Pamuku⁴; Stephen Benchouk⁵; ¹Duquesne University, Pittsburgh, PA; ²Agilent Technologies, Inc., Santa Clara, CA; ³GERSTEL, Inc., Linthicum, MD; ⁴Applied Isotope Technologies Company, Pittsburgh, PA; ⁵Infinity Life Center, Honolulu, HI
- WP 131 **Analytical Method Development for Widely Targeted Perfluoroalkyl Acids (PFAAs) and their Precursors in Plasma using Multi-Gradient Eluent System by LC-MS/MS**; Jun Watanabe¹; Toshikazu Minohata¹; Tairo Ogura²; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instr., Columbia, MD
- WP 132 **An APGC-MS MRM Method for the Quantitation of Common Acrylates in a Single Method**; Vincent Pagnotti¹; Benjamin Cooley¹; Conner Stultz²; Frank Dorman²; ¹PPG Industries, Allison Park, PA; ²Pennsylvania State University, State College, PA
- WP 133 **Materials and Methods for Measuring the Non-Protein Amino Acid BMAA in Proteins**; David C Muddiman¹; Philip L Loziuk¹; Lauren C Nufer¹; Yasamin Moazami¹; Joshua G Pierce¹; Denis Fourches¹; Scott J Mellors²; J. Michael Ramsey³; ¹North Carolina State University, Raleigh, NC; ²908 Devices, Inc., Carrboro, NC; ³UNC, Chapel Hill, NC
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- UPLC/MSE Platform and Progenesis QIP with Spectral Library;** Joanne Cotton¹; Martha Stapels¹; Lin Liu¹; Dongyu Liu¹; Clarence Wang¹; Ian Reah²; Steven Anderson²; Ian Morns²; Xiaoying Jin¹; ¹Sanofi, Framingham, MA; ²Waters Corporation, Newcastle upon Tyne, UK
- WP 227 **High-Detail Analysis of Plasma Glycoprotein Microheterogeneity by Hybrid Mass Spectrometry Approaches;** Vojtech Franc¹; Yang Yang¹; Albert J. R. Heck¹; ¹Utrecht University, Utrecht, NE
- WP 228 **Effect of Sialic Acids on N-glycan Release Kinetics by PNGase F;** Naglaa Sheiba¹; Ron Orlando¹; ¹CCRC, University of Georgia, Athens, GA
- WP 229 **Quantitative Glycoproteomics in Complex Samples using Soft Fragmentation;** Miloslav Sanda¹; Petr Kozlik^{1,2}; Nathan J Edwards³; Radoslav Goldman^{1,3}; ¹Georgetown University, Lombardi Cancer Center, Washington, DC; ²Charles University, Faculty of Science, Department of Analytical Chemistry, Prague, Czech Republic; ³Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC
- WP 230 **Development of a Novel Glycoproteomics Tool, Glycopeptide Decoy Generator, for Determining the Accuracy of Algorithms that Assign Glycopeptide CID Data;** Jude Lakub¹; Xiaomeng Su¹; Zhikai Zhu¹; David Hua¹; Eden Go¹; Heather Desaire¹; ¹University of Kansas, Lawrence, KS
- WP 231 **In-Depth Site-Specific Glycan Microheterogeneity Characterization with Reversed-Phase Chromatographic Prefractionation Followed by Capillary Zone Electrophoresis-Electrospray Ionization Tandem Mass Spectrometry Analysis;** Yanyan Qu¹; Liangliang Sun²; Zhenbin Zhang¹; Norman J Dovichi¹; ¹Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; ²Department of Chemistry, Michigan State University, East Lansing, MI
- WP 232 **Facile and Selective Enrichment of Intact Sialoglycopeptides Using Graphitic Carbon Nitride without Dephosphorylation of Peptides;** Mo Zhang¹; Yujie Liu¹; Dan Zhang¹; Tianjing Cheng¹; Zhili Li¹; ¹Institute of Basic Medical Sciences, CAMS & PUMC, Beijing
- WP 233 **pGlyco 2.0 Enables Precision Glycoproteomics by using Comprehensive Quality Control and One-Step Mass Spectrometry for Intact Glycopeptide Identification;** Mingqi Liu¹; Wen-Feng Zeng²; Wei-qian Cao¹; Chao Liu²; Si-Min He²; Peng-Yuan Yang¹; ¹Fudan University, Shanghai, China; ²Key Lab of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Beijing, China
- WP 234 **Enhancing Glycopeptide MS Performance through Derivatization with a Novel Rapid Derivatization Reagent;** William Alley¹; Brad Williams²; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA
- WP 235 **Deep Sequencing of Proteoglycans;** Le Meng¹; Joshua A. Klein²; Joseph Zaia¹; ¹Boston University School of Medicine, Boston, MA; ²Boston University, Boston, MA
- WP 236 **Identification of Sialic Acid Linkages using Esterification on Solid-Phase;** Shuang Yang¹; Ewa Jankowska¹; Lisa M Parsons¹; John F Cipollo¹; ¹Food and Drug Administration/ CBER, Silver Spring, MD
- WP 237 **Evaluation of Electron Transfer Dissociation Reagents for Analysis of N-Glycosylated Peptides;** Maia I. Kelly¹; Eric D. Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- WP 238 **Site-Specific MS-Based Characterization of Complex Glycoproteins using HILIC and Reversed-Phase Chromatography;** Gordon R. Nicol¹; Brian Gau¹; Amber Henry¹; Kevin Ray¹; ¹MilliporeSigma, St Louis, MO
- WP 239 **Microwave-Assisted Immobilized Enzyme Reactors Preparation for Rapid Offline Peptide, Glycan, and Glycopeptide Sample Preparation;** Kerry Wooding¹; Alireza Banazadeh¹; Chengyuan Liu¹; Dalia Khater¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 240 **Top-Down Sequencing and N-Glycosylation Site Mapping by Ultrahigh Resolution 21 Tesla FT-ICR MS/MS;** Tingting Jiang¹; Lissa C. Anderson²; Christopher L Hendrickson^{1,2}; Alan G. Marshall^{1,2}; ¹Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; ²Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL
- WP 241 **LC-MS Based Analysis of Underivatized N-Glycans Released from a Prostate Cancer-Related Glycoprotein;** Abby S. Gelb¹; Christine Booth¹; Katherine N. Schumacher¹; Melanie A. Simpson¹; Eric D. Dodds¹; ¹University of Nebraska-Lincoln, Lincoln, NE
- WP 242 **Library Based Automated Glycan Identification by Mass Spectrometry in Combination with Fluorescence Quantification;** Robert Wilmanowski¹; Sven Bahrke¹; Detlev Suckau²; Wolfgang Jabs³; ¹Glycotope GmbH, Berlin, Germany; ²Bruker Daltonik GmbH, Bremen, Germany; ³Beuth University of Applied Sciences Berlin, Berlin, Germany
- WP 243 **Enhanced Enrichment and Analysis of Glycopeptides From Whole Gut Lavage Fluid Using Off-line HILIC HPLC Chromatography and C18 LC- MS/MS;** Crystal Daniels¹; Lewis K. Pannell¹; Joseph Otto¹; ¹Mitchell Cancer institute, Mobile, AL
- WP 244 **Mass Spectrometry Characterization of Trehalose Glycopolymer and its Insulin Conjugate;** Sahar Sallam¹; Chrys Wesdemiotis¹; Yang Liu²; Juneyoung Lee²; Jeong Hoon Ko²; Kathryn Mansfield²; Heather Maynard²; ¹The University of Akron, Akron, OH; ²University of California, Los Angeles, Los Angeles, CA
- WP 245 **Applying a Novel Informatics Approach to Study Site-Specific Urinary Protein N-Glycosylation in the Context of Urinary Tract Infection (UTI);** John Froehlich^{1,2}; Peter Warren¹; Shannon DiMartino¹; Richard S Lee^{1,2}; ¹Boston Children's Hospital, Boston, MA; ²Harvard Medical School, Boston, MA
- WP 246 **Quantitation of Human Antibodies with Synthetic Glycopeptides;** Rini Roy¹; Emy Komatsu¹; Helene Perreault¹; ¹University of Manitoba, Winnipeg, MB
- WP 247 **Profiling of Site-specific N-Glycosylation in Human Serum by Analyses of N-linked Glycans And Glycosite-containing Peptides (NGAG) ;** Shisheng Sun^{1,2}; Yingwei Hu¹; Shadi Toghi Eshghi¹; Yang Liu¹; PUNIT SHAH¹; Jing Chen¹; Hui Zhang¹; ¹Johns Hopkins University, Baltimore, MD; ²Northwest University, Xi'an, China
- WP 248 **Analysis of Clustered Activity of GalNAc-T2 on IgA1 Hinge Region Reveals New Roles for Initial Glycan Position on Subsequent Glycosylation;** Tyler Stewart¹; Kazuo Takahashi²; Milan Raska³; Robert H. Whitaker¹; William J. Placzek¹; Jan Novak¹; Matthew B. Renfrow¹; ¹University of Alabama at Birmingham, Birmingham, AL; ²Fujita Health University School of Medicine, Toyooka, Japan; ³Palacky University, Olomouc, Czech Republic
- WP 249 **Separation and Characterization of Fab and Fc Fragments from Swine Immunoglobulin G (IgG) Papain Digests by MALDI-MS;** Claudia Nelson¹; Emy Komatsu¹; Helene Perreault¹; ¹University of Manitoba, Winnipeg, MB
- WP 250 **Automated Preparation of Labeled N-Glycans with a Vision-Guided Pipetting Robot for High Sensitivity LC-MS Analysis;** Stephan Koza¹; Corey E Reed¹; Nikolas Vamvoukas²; Erin Chambers¹; ¹Waters Corp, Milford, MA; ²Andrew Alliance S. A., Geneva, Switzerland
- WP 251 **An Efficient Targeted Analysis Approach for Full N-Glycosylation Site Mapping of Highly Glycosylated Proteins and/or Glycoprotein Mixtures;** Milani R. Wijeweera Patabandige¹; Eden P. Go¹; Heather Desaire¹; ¹University of Kansas, Lawrence, KS



WEDNESDAY POSTERS

- WP 252 **Bioinformatics-Assisted Discovery of Altered Glycotopes on Serum Protein in Hepatocellular Carcinoma**; Ta-Chi Yen^{1,2}; Yi-Ju Chen²; Yu-Ju Chen²; ¹Genome and Systems Biology Degree Program, National Taiwan University, Taipei, Taiwan; ²Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- WP 253 **Reliable Quantitative Analysis of N-linked Glycopeptides Derived from Cancer Cells by Metabolic Isotopic Labeling**; Jingfu Zhao¹; Wenjing Peng¹; Joshua M. Gutierrez¹; Alex Harvey²; Barry Boyes²; Ron Orlando²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²GlycoScientific, LLC, Athens, GA
- WP 254 **Carbohydrate Sequencing Complete with Spectral Documentation by MSn**; Vernon Reinhold¹; Qing Guo²; David Ashline²; ¹University of New Hampshire, Durham, NH; ²University of New Hampshire, Durham, NH

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- WP 255 **Development of an Internal Exchange Standard for Gas-phase Hydrogen/Deuterium Exchange Mass Spectrometry**; Sanjit S Uppal¹; Sarah E Beasley¹; Miklos Guttman¹; ¹Department of Medicinal Chemistry, University of Washington, Seattle, WA
- WP 256 **Discrimination of Isomeric Glycans by Gas-Phase Hydrogen/Deuterium Exchange**; Sanjit Uppal¹; Sarah Beasley¹; Michele Scian¹; Miklos Guttman²; ¹University of Washington, Department of Chemistry, Seattle, WA; ²University of Washington, Seattle, WA
- WP 257 **Evolution and Evaluation of a Modular Automation Platform for HDX MS**; Alfonso Espada¹; Ruben Haro¹; Cristina Sayago¹; Jesus Castanon¹; Bruce D pascal²; Patrick R Griffin²; Jeffrey A. Dodge³; Michael J Chalmers⁴; ¹Lilly S.A., Alcobendas, Madrid; ²The Scripps Research Institute, Jupiter, FL; ³Eli Lilly and Company, Indianapolis, IN; ⁴Eli Lilly and Company, Indianapolis, IN
- WP 258 **Antibody Aggregate Interface Mapping by Hydrogen Deuterium Exchange Mass Spectrometry using a Customized Automation Instrument**; Qian Zhang¹; Hui Xiao¹; Shailin Patel¹; Chen Li¹; Ning Li¹; ¹Regeneron Pharmaceuticals, Tarrytown, NY
- WP 259 **Optimizing Electron Transfer Dissociation Conditions for Hydrogen/Deuterium Exchange Mass Spectrometry and Its Application to the Study of Protein Conformation**; Terry Zhang¹; Stephane Houel²; Jonathan Josephs¹; ¹ThermoFisher, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA
- WP 260 **Comparison of Immobilized Nepenthesin II and Pepsin Cleavage Specificities in HDX-MS Conditions**; Bruce D. Pascal¹; Venkatasubramanian Dharmarajan¹; Jie Zheng¹; Adrian Reich¹; Ruben Garcia-Ordóñez¹; Scott Novick¹; Patrick R Griffin¹; ¹The Scripps Research Institute, Jupiter, FL
- WP 261 **Higher Selectivity Digestion Strategies for the HX-MS Analysis of Large Protein Constructs**; Joey Sheff¹; Christoph Schröder²; Linda Lee²; David C. Schriemer²; ¹University of Calgary, Calgary, AB, Canada; ²University of Calgary, Calgary, AB, Canada
- WP 262 **An Operational Platform for Proteolytic Hydrogen-Deuterium Exchange Mass Spectrometry that Conducts Chromatographic Separations at -30°C**; Jeffrey W. Huddgens^{1,2}; Kyle W. Anderson^{2,3}; Ioannis Karageorgos^{2,3}; ¹National Institute of Standards and Technology, Rockville, MD; ²Institute for Bioscience and Biotechnology Research, Rockville, MD; ³NIST, Gaithersburg, MD
- WP 263 **Sparse Representation for Hydrogen Exchange Mass Spectrometry (HX-MS) Data by using LASSO Optimization**; Yugi Shi¹; Jarod V. Hart^{2,3}; David D. WEIS^{1,4}; ¹Department of Chemistry, University of Kansas, Lawrence, KS; ²Higuchi Biosciences center, University of Kansas,

- Lawrence, KS; ³Department of Mathematics, University of Kansas, Lawrence, KS; ⁴Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS
- WP 264 **Characterizing the Forward- and Backward- Hydrogen/Deuterium Exchange of Hydroxyls Resulting from Residual Solvent Vapors in Electrospray Sources**; H. Jamie Kim¹; Marina R. Mullenos¹; Tara Liyanage¹; Elyssia S Gallagher¹; ¹Baylor University, Waco, TX
- WP 265 **Paradigm Shift of HDX-MS Data Analysis: From Centroid Values and Deuteration Levels to Isotope Envelopes and Exchange Rates**; Yoshitomo Hamuro; Consultant, Lawrenceville, NJ
- WP 266 **Peptide-Level HDX Analysis of Denatured Insulin is a Model Assay for Therapeutic Protein Structural Fidelity**; Elizabeth T. Schaper Bergman¹; Henry W. Rohrs¹; Michael L. Gross¹; ¹Washington University, Saint Louis, MO
- WP 267 **Automated Hydrogen-Deuterium Exchange Analysis of Intact Proteins by Top-Down Fragmentation using Electron Transfer Dissociation**; Malcolm Anderson¹; Laetitia Florence Denbigh¹; Keith Fadgen²; Michael Eggertson²; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; ²Waters Corp, Milford, MA
- WP 268 **An Empirical Method to Correct for Altered Chemical Exchange Effects in Hydrogen Exchange-Mass Spectrometry (HX-MS)**; Ronald T. Toth¹; Sangeeta B. Joshi²; Reza Esfandiary³; C. Russell Middaugh¹; David B. Volkin²; David Weis⁴; ¹University of Kansas, Lawrence, KS; ²University of Kansas, Lawrence, KS; ³Medimmune LLC, Gaithersburg, Maryland; ⁴University of Kansas, Lawrence, KS
- WP 269 **Probing Membrane Protein Conformational Dynamics using HDX-MS**; Yingrong Xu¹; Jill Chrencik¹; Kimberly F. Fennell¹; Laura Byrnes¹; Justin Hall¹; Xiayang Qiu¹; Graham West¹; ¹Pfizer Inc., Groton, CT
- WP 270 **Combined HDX ETD Workflow for Increasing Spatial Resolution in Higher Order Structure Study**; Ying-Qing Yu¹; Jing Fang¹; Michael Eggertson¹; Keith Fadgen¹; Weibin Chen¹; ¹Waters Corp, Milford, MA
- WP 271 **Hydrogen/Deuterium Exchange Analysis Aimed at Parameter Optimization for High Resolution FT-ICR MS Instruments**; Greg T. Blakney¹; Lissa Anderson¹; Yuri E Corilo¹; Peilu Liu²; Alan G. Marshall^{1,2}; Chad R Weisbrod¹; Christopher L Hendrickson^{1,2}; ¹National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ²Florida State University, Tallahassee, FL
- WP 272 **Low Temperature Hydrogen Exchange Microchip Capillary Electrophoresis-Mass Spectrometry**; Kristina M. Herrera¹; J. Michael Ramsey¹; ¹UNC - Chapel Hill, Chapel Hill, NC
- WP 273 **Supercharging for Improved ECD/ETD-Based Hydrogen/Deuterium Exchange Mass Spectrometry**; Qingyi Wang¹; Kristina I Håkansson¹; ¹University of Michigan Chemistry Department, Ann Arbor, MI
- WP 274 **Mass Spectrometry Measurements of the Isotope Ratios of Low Abundant Glycated Peptides**; Sergei Ilchenko¹; Kwangwon Lee²; Takhar Kasumov²; ¹Northeast Ohio Medical University, Rootstown, OH; ²Northeast Ohio Medical University, Rootstown, OH

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- WP 275 **Steering Biological Discovery Through Multimodal Imaging with Mass Spectrometry Using Data-driven Image Fusion**; Raf Van de Plas^{1,2,3}; Jeffrey Spraggins^{2,3}; Nico Verbeeck¹; Boone M. Prentice^{2,3}; William J. Perry^{2,4}; Junhai Yang^{2,3}; Martina Marchetti-Deschmann⁵; Eric P. Skaar^{6,7}; Richard M. Caprioli^{2,3,4,8,9}; ¹Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department



of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Chemistry, Vanderbilt University, Nashville, TN; ⁵Institute of Chemical Technologies and Analytics (CTA), TU Wien, Vienna, Austria; ⁶Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; ⁷United States (U.S.) Department of Veterans Affairs, Tennessee Valley Healthcare System, Nashville, TN; ⁸Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁹Department of Medicine, Vanderbilt University, Nashville, TN

- WP 276 **Data Directed Mass Spectrometry Imaging – Real Time Decision Making during Automated Analysis of Sample Slide Batches;** Emrys Jones^{1,2}; Emmy Hoyes¹; Lukasz Migas³; Fiona Henderson⁴; Praveen Harapanahalli¹; Richard Chapman¹; Adam McMahon³; Steven Pringle¹; Zoltan Takats²; ¹Waters Corporation, Wilmslow, UK; ²Imperial College London, London, London; ³University of Manchester, Manchester, UK; ⁴University of Manchester, Manchester, UK
- WP 277 **Blind Source Separation of MALDI Spectra from Noise by Sparse Representation in a Composite of Linear Bases;** Luis Mancera¹; Luis A. González-Jaime¹; Matthew Openshaw²; ¹Clover Bioanalytical Software; ²Shimadzu, Manchester, UK
- WP 278 **Practical Considerations for Multicenter Studies: Software Tools for Managing Large Cohorts of MALDI Imaging Data;** Fingal Orlando Galashan¹; Jan Hendrik Kobarg¹; Stefan Frehse¹; Janina Oetjen²; Rita Casadonte³; Delf Lachmund⁴; Klaus Steinhorst¹; Stefan Schiffler¹; Tobias Boskamp^{1,4}; Peter Maass⁴; Joerg Kriegsmann^{3,5}; Theodore Alexandrov^{6,7}; Dennis Trede¹; ¹SciLS GmbH, Bremen, Bremen; ²MALDI Imaging Lab, University of Bremen, Germany; ³ProteoPath GmbH, Trier, Germany; ⁴Center for Industrial Mathematics, University of Bremen, Germany; ⁵Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany; ⁶EMBL, Heidelberg, Baden-Wuerttemberg; ⁷Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA
- WP 279 **Distilling Knowledge from Data: MS Data Analysis using ChemDistiller;** Ivan Laponogov¹; Nouredin M H Sadawi¹; Dennis A Veselkov¹; Dieter Galea¹; Kirill A Veselkov¹; ¹Imperial College London, London, UK
- WP 280 **Advanced Computer Vision Based Registration of Imaging Mass Spectrometry Data in Multi-Modal Experiments;** Nico Verbeeck¹; Jeffrey Spraggins^{2,3}; Nathan Heath Patterson^{2,3}; Junhai Yang^{2,3}; Etienne Waelkens^{5,6}; Richard M. Caprioli^{2,3,4,7,8}; Raf Van de Plas^{1,2,3}; ¹Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Mass Spectrometry Research Center (MSRC), Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Chemistry, Vanderbilt University, Nashville, TN; ⁵Dept. of Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; ⁶Sybioma, KU Leuven, Leuven, Belgium; ⁷Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁸Department of Medicine, Vanderbilt University, Nashville, TN

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- WP 281 **Rapid 500 nm-Resolution Imaging of the Cellular Lipidome in Model Neurons by TOF-SIMS Parallel Imaging MS/MS;** Gregory L Fisher¹; Rachelle Balez²; Anne L Bruinen³; Ron MA Heeren³; Lezanne Ooi²; ¹Physical Electronics, Chanhassen, Minnesota; ²School of Biological Sciences, The University of Wollongong, Wollongong, Australia; ³Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands

- WP 282 **Improved Spatial Resolution IR-MALDESI Mass Spectrometry Imaging;** Mark Bokhart¹; Jeffrey Manni²; Måns Ekelöf¹; Milad Nazari¹; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²JGM Associates Inc., Burlington, MA
- WP 283 **Pushing the Limits of DESI-FTICR MS Imaging using Advanced Data Acquisition and Processing Approaches;** Pieter C. Koopman¹; Anton N. Kozhinov²; Konstantin O. Nagornov²; David P.A. Kilgour³; Yury O. Tsybin²; Ron M.A. Heeren¹; Shane R. Ellis¹; ¹Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; ²Spectroswiss Sàrl, Lausanne, Switzerland; ³Nottingham Trent University, Nottingham, UK
- WP 284 **A Pneumatically Assisted Nanospray Desorption Ionization (nano-DESI) Source for Enhanced Metabolite Imaging from Tissue;** Kyle D Duncan¹; Hilde-Marlene Bergman¹; Ingela Laneckoff¹; ¹Uppsala University, Uppsala, Sweden
- WP 285 **High-Resolution Tissue Imaging Using Subatmospheric and Atmospheric MALDI sources;** Eugene Moskovets¹; Shelley N. Jackson²; Ludovic Muller²; Damon Barbacci³; Vladimir Doroshenko¹; J. Albert Schultz³; Amina S. Woods²; ¹MassTech Inc, Columbia, MD; ²NIDA-IRP, NIH, Baltimore, MD; ³Ionwerks, Inc., Houston, TX
- WP 286 **TOF-SIMS and MS/MS Parallel Imaging Instrumentation for Sub-Micron Molecular Characterization;** GREGORY L FISHER¹; Paul E. Larson¹; John S. Hammond¹; Scott Bryan¹; ¹Physical Electronics, Chanhassen, MN
- WP 287 **Development of an Imaging FT-ICR-MS with SIMS, FIB-SEM, and Post-Ionization Capabilities for Biological Applications;** Matthew Brantley¹; Ian G. M. Anthony¹; Raul A. Villacob¹; Carter Lantz¹; Adam R. Floyd¹; Christina A. Gaw¹; Scott Koziol¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- WP 288 **Development of an Optical System for Uniform Laser Irradiation in Stigmatic Imaging Mass Spectrometry;** Yuma Tsurumoto¹; Hisanao Hazama¹; Kunio Awazu^{1,2}; ³Graduate School of Engineering, Osaka University, Suita, Japan; ²Graduate School of Frontier Biosciences, Osaka University, Suita, Japan; ³Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan
- WP 289 **A Monte-Carlo Approach To Automated Ion Trajectory Calculations for Optimization of an Imaging FT-ICR MS with Post-Ionization Capabilities;** Raul Villacob¹; Matthew R. Brantley¹; Ian G.M. Anthony¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- WP 290 **Simultaneous Imaging of Small Metabolites, Lipids and Proteins from Biological Tissues under Ambient Conditions Using Laser Electrospray Mass Spectrometry;** Fengjian Shi¹; Rachel J. Parise¹; Evan M. Lutton²; Servio H. Ramirez²; Robert J. Levis¹; ¹Department of Chemistry, Temple University, Philadelphia, PA; ²Lewis Katz School of Medicine, Temple University, Philadelphia, PA
- WP 291 **Multimodal Chemical and Functional Imaging of Nanoscale Transformations in Ferroelectric Thin Films;** Anton Levlev¹; Chance C. Brown²; Petro Maksymovych²; Sergei V. Kalinin²; Olga S. Ovchinnikova²; ¹Oak Ridge National Lab, Oak Ridge, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN

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- WP 292 **A Critical Way of Optimizing Tissue Microarrays (TMAs) Sample Preparation Compatible with Mass Spectrometry Imaging;** Michele Genangeli^{1,2}; Stacey Meulenberg²; Lindsay Hewitt³; Heike Grabsch³; Sauro Vittori¹; Benjamin Balluff²; Ron Heeren²; Tiffany Porta²; ¹University of Camerino - Unicam, Camerino (MC), Italy; ²Maastricht Multi-Modal Molecular Imaging (M4I) Institute,



- WP 293 **Improvements in Mass Spectrometry Imaging for the Molecular Analysis of FFPE Tissue Sections;** Alice Ly¹; Rita Casadonte²; Mark Kriegsmann³; Joerg Kriegsmann²; Michael Becker^{1,4}; Juergen Tressel¹; Soeren-Oliver Deininger¹; ¹Bruker Daltonics, Bremen, Germany; ²ProteoPath GmbH, Trier, Germany; ³University of Heidelberg, Heidelberg, Germany; ⁴Boehringer Ingelheim GmbH, Biberach, Germany
- WP 294 **Assessing Imaging Compatibility and Performance of Various Tissue Fixation Strategies using MALDI FTICR MS;** Marissa Jones¹; Jeffrey M. Spraggins^{2,3,4}; Nathan Heath Patterson^{2,4}; William Perry^{2,3}; Richard M. Caprioli^{2,3,4,5,6}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department of Chemistry, Vanderbilt University, Nashville, TN; ⁴Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN
- WP 295 **Phosphopeptide enhancement in MALDI IMS Experiments;** Hyojik Yang^{1,2}; Jeremy L. Norris^{1,2,3}; Kevin L. Schey^{1,2}; Jeffrey Spraggins^{1,2,3}; Richard M. Caprioli^{1,2,3,4}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Biochemistry, Vanderbilt University, Nashville, TN; ³Department of Chemistry, Vanderbilt University, Nashville, TN; ⁴Department of Pharmacology and Medicine, Vanderbilt University, Nashville, TN
- WP 296 **Modified TiO₂ Monolith for Selective Imprint Imaging of Brain Tissue by Laser Desorption/Ionization-Mass Spectrometry;** Qian Wu¹; Stanislav S. Rubakhin¹; Jonathan V. Sweedler¹; ¹Department of Chemistry and the Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL
- WP 297 **Understanding the Laser Desorption Ionization Mechanisms of Lipids from Tissue Sections After Matrix Deposition by Sublimation;** Nicolas Elie¹; Sebastiaan Van Nuffel¹; Alain Brunelle¹; Pierre Chaurand^{1,2,3}; ¹CNRS, Institut de Chimie des Substances Naturelles, Gif sur Yvette, France; ²University of Montreal, Montreal, QC, Canada; ³Université Paris-Saclay, Saint-Aubin, France
- WP 298 **Insect Neuropeptide MALDI Imaging: Simultaneous Analysis and Localization with Spatial Resolution at Micrometer Scale;** Alice Ly¹; Lapo Ragonieri²; Sander Liessem²; Michael Becker^{3,4}; Soeren-Oliver Deininger³; Reinhard Predel²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²University of Cologne, Cologne, Germany; ³Bruker Daltonics, Bremen, Germany; ⁴Boehringer Ingelheim GmbH, Biberach, Germany
- WP 299 **Visualization of Glucosinolate Distribution in the Inner Structure of the Leaf by Mass Spectrometry Imaging;** Tomomi Ichinose¹; Fusa Murayama¹; Yoshinori Fujimura¹; Yuzo Yamazaki²; Hiroyuki Wariishi¹; Akiko Maruyama¹; Daisuke Miura¹; ¹Kyushu University, Fukuoka, Japan; ²Shimadzu, Kyoto, Japan
- WP 300 **Matrix-Enhanced SIMS Depth Profiling to Probe the Matrix Extraction Efficiency and Distribution of Drugs in Brain, Liver, and Intestinal Tissue;** Joel Keeler¹; Lennart Huizing¹; Arnoud Prop¹; Anne L. Bruinen¹; Shane R. Ellis¹; Rob Vreeken^{1,2}; Ron MA Heeren¹; ¹Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; ²Janssen R&D, Beerse, Belgium
- WP 301 **Surface Layer-MALDI MS-Imaging of Polymer Film Defects and Segregation;** Kevin J. Endres¹; Jacob A. Hill¹; Mark D. Foster¹; Chrys Wesdemiotis¹; ¹University of Akron, Akron, OH
- WP 302 **Sample Preparation of the Corn Seed Tissues to Prevent Analyte Relocations for MS imaging;** Sohee Yoon¹; Shin-Hye Kim¹; Tae Geol Lee¹; Jeongkwon Kim²; ¹Korea Research Institute of Standards and Science, Daejeon; ²Chung Nam National University, Daejeon, South Korea
- WP 303 **Global Lipidomic Changes Associated with MALDI Matrices using MALDI FTICR Imaging Mass Spectrometry;** William J. Perry^{1,2}; Jeffrey M. Spraggins^{2,3}; Raf Van de Plas^{1,3,4}; Richard M. Caprioli^{1,2,3,5,6}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Chemistry, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN
- WP 304 **Establishment of Convenient Sample Preparation Method with High Sensitivity and Excellent Reproducibility in Mass Spectrometry Imaging of Endogenous Primary Metabolites;** Tomomi Ichinose¹; Fusa Murayama¹; Takanori Ishii¹; Chihiro Kawano¹; Ayaka Murayama¹; Akiko Miki¹; Yoshinori Fujimura¹; Yuzo Yamazaki²; Hiroyuki Wariishi¹; Daisuke Miura¹; ¹Kyushu University, Fukuoka, Japan; ²Shimadzu Corporation, Kyoto, Japan
- WP 305 **Ketone Based Matrices for Imaging Proteins;** Junhai Yang^{1,2}; Richard M. Caprioli^{1,3}; ¹Department of Biochemistry, Vanderbilt University, Nashville, TN; ²The Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Chemistry, Pharmacology and Medicine, the Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN
- WP 306 **Caffeic Acid as a New Matrix for Enhanced Tissue Imaging of High Molecular Weight Proteins by MALDI Mass Spectrometry;** Xiaodong Wang¹; Huixin He¹; Liang Qin¹; Lulu Chen¹; Yaqin Liu¹; ¹Centre for Imaging & Systems Biology, College of Life and Environmental Sciences, Minzu University of China, Beijing, China

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- WP 308 **3D ToF-SIMS Imaging of Cells;** Daniel J. Graham¹; Lara J. Gamble¹; ¹University of Washington Department of Bioengineering, Seattle, WA
- WP 309 **Uranium Bearing Particle Identification using a Fully Convolutional Neural Network and Watershed Segmentation;** Jay Tarolli¹; ¹Pacific Northwest National Laboratory, Richland, WA
- WP 310 **Novel Data Analysis Approaches for Mass Spectrometry Imaging Multicenter Studies;** Stefan Frehse¹; Jan Hendrik Kobarg¹; Vitaly Kovalev²; Fingal Orlando Galashan¹; Stefan Schifferl¹; Klaus Steinhorst¹; Tobias Boskamp^{1,3}; Andrew Palmer²; Rohan A. Thakur⁴; Theodore Alexandrov^{1,2,5}; Dennis Trede^{1,4}; ¹SCiLS GmbH, Bremen; ²EMBL, Heidelberg, Heidelberg; ³University of Bremen, Bremen, Germany; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵University of California, San Diego, CA
- WP 311 **Real-Time Viewing, Classification and 3D Reconstruction for Imaging Mass Spectrometry;** Richard Chapman¹; Emrys Jones¹; Csaba Hajdu²; Emmy Hoyes¹; Praveen Harapanahalli¹; Emmanuelle Claude¹; Robert Tonge¹; Steven Pringle¹; ¹Waters Corporation, Wilmslow, UK; ²Waters Research Center, Budapest



- WP 312 **Mass Spectrometry Image Exploration and Annotation with MSiReader**; Kenneth Garrard¹; Milad Nazari¹; Mark Bokhart¹; Måns Ekelöf¹; Sitora Khodjanizova¹; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC

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- WP 314 **Specter: Deconvolution of Data Independent Acquisition Mass Spectrometry Data by Linear Regression of Acquired Spectra onto Libraries**; Ryan Peckner¹; Samuel A Myers¹; Jarrett Egertson²; Richard S Johnson²; Michael J MacCoss²; Jacob D Jaffe¹; ¹Broad Institute, Cambridge, Massachusetts; ²University of Washington, Seattle, WA
- WP 315 **Philosopher: A Data Processing Toolkit for Shotgun Proteomics**; Felipe da Veiga Leprevost¹; Avinash Kumar Shanmugam¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
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- WP 317 **Discriminating Isobaric Phosphopeptides using Data-Independent Acquisition Mass Spectrometry**; Zuofei Yuan¹; Simone Sidoli¹; Rina Fujiwara¹; Katarzyna Kulej^{1,2}; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA; ²The Children's Hospital of Philadelphia, Philadelphia, PA
- WP 318 **An Ion Library-Free, Data Independent Acquisition Strategy for Vibrio natriegens Proteome Characterization using Deep DIA's DeepSearch Protocol**; William Judson Hervey, IV¹; Gautam Saxena²; Krystine Pimentel³; Gary J. Vora⁴; ¹Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC; ²DeepDIA, Bethesda, MD; ³Department of Computer and Electrical Engineering, Florida International University, Miami, FL; ⁴Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC
- WP 319 **Quantifying Phosphopeptide Positional Isomers in DIA Experiments**; Brian C. Searle^{1,2}; Michael J. MacCoss¹; Judit Villén¹; ¹University of Washington, Department of Genome Sciences, Seattle, WA; ²Proteome Software, Portland, OR
- WP 320 **TargetedMSQC: An R Package for Peak Quality Assessment and Interference Detection in Targeted Mass Spectrometry Proteomics Datasets**; Shadi Toghi Eshghi¹; Kristin Wildsmith¹; Paul Auger¹; W. Rodney Mathews¹; ¹Genentech, South San Francisco, CA
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- WP 322 **Protecting Proteomic Data Processing on the TDPortal with the Open Science Cyber Risk Profile**; Richard Leduc¹; Ryan T. Fellers²; Joseph B. Greer²; Jackie Milhans²; Von Welch³; Paul Thomas²; Neil L Kelleher²; ¹Northwestern University, Bloomington, Indiana; ²Northwestern University, Evanston, IL; ³Indiana University, Bloomington, IN

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- WP 325 **Metandem: A Novel Online Software Platform for Mass Spectrometry-Based Isobaric Labeling Metabolomics**; Ling Hao¹; Pingli Wei¹; Fabao Liu²; Jillian Johnson¹; Amanda Buchberger¹; W. John Kao³; Wei Xu²; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI; ²McArdle Laboratory for Cancer Research, UW-Madison, WI; ³President's Office, the University of Hong Kong, Hong Kong, China
- WP 326 **DeltaMS: A Convenient Tool to Track Isotopologues in GC/LC-MS Data by Stable Isotope Probing (SIP)**; Tim Baumeister¹; Nico Ueberschaa²; Wolfgang Schmidt-Heck³; Jan-Frieder Mohr²; Michael Deicke²; Thomas Wichard²; Reinhard Guthke³; Georg Pohnert^{1,2}; ¹Max Planck Institute for Chemical Ecology, Max Planck Fellow Group Plankton Community Interaction, Jena, Germany; ²Friedrich Schiller University Jena, Jena, Germany; ³Leibniz Institute for Natural Product Research and Infection Biology – Hans Knoll Institute (HKI), Department of Systems Biology and Bioinformatics, Jena, Germany
- WP 327 **Metabolite Annotations for Spectra Not Available in Spectral Library via In Silico Molecular Networking and Raw Data Spectral Matching**; Ricardo Silva¹; Alexandria Ongjoco²; Pieter C. Dorrestein^{3,4}; ¹University of California, San Diego, CA; ²Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA; ³Skaggs School of Pharmacy, University of California San Diego, San Diego, CA; ⁴Department of Pediatrics, University of California San Diego, San Diego, CA
- WP 328 **New Algorithms for Reducing the Rate of False Positive and False Negative Compounds Detected from Mass Spectrometry Metabolomics Data**; Owen Myers¹; Susan Sumner²; Shuzhao Li³; Stephen Barnes⁴; Xiuxia Du¹; ¹University of North Carolina at Charlotte, Charlotte, NC; ²University of North Carolina at Chapel Hill, Chapel Hill, NC; ³Emory University, Atlanta, Georgia; ⁴University of Alabama at Birmingham, Birmingham, AL
- WP 329 **MetabVision: A Shiny Based Web Framework for Quality Control (QC), Data Normalization and Visualization in Untargeted Metabolomics**; Tanu Soni¹; Matthew Hansen²; Charles Evans^{1,3}; Sarah Tishkoff²; Charles Burant^{1,3}; Thekkelnayck Rajendiran^{1,4}; ¹Michigan Regional Comprehensive Metabolomics Resource Core, University of Michigan, Ann Arbor, MI; ²Departments of Genetics and Biology, University of Pennsylvania, Philadelphia, PA; ³Department of Internal Medicine, University of Michigan, Ann Arbor, MI; ⁴Department of Pathology, University of Michigan, Ann Arbor, MI
- WP 330 **Automatic Pipeline Package for Identification and Normalization of LCMS-Based Untargeted Metabolomics**; Chuan-Yih Yu¹; Johannes Fahrman¹; Eunice Murage¹; Jennifer Dennison¹; Samir Hanash¹; ¹MD Anderson Cancer Center, Houston, TX
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- WP 332 **A Web Service Framework for Interactive Browsing of Metabolomics Data**; Yaroslav Lyutvinskiy¹; Jeramie Watrous²; Mohit Jain²; Roland Nilsson¹; ¹Karolinska institute, CMM, Stockholm, Sweden; ²UCSD, La Jolla, CA
- WP 333 **Galaxy-Centered Lab Workflows to Organize Metabolomic Analyses**; Arthur C. Eschenlauer^{1,2,3}; Mark Esler^{1,3}; Jerry D. Cohen^{1,3}; Timothy J. Griffin^{2,4}; Adrian D. Hegeman^{1,3}; ¹Microbial and Plant Genomics Institute and Dept. of Horticultural Science, University of Minnesota, St. Paul, MN; ²Dept. of Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, Minneapolis, MN; ³University of Minnesota, St. Paul, MN; ⁴University of Minnesota, Minneapolis, MN
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- WP 335 **Artificial Neural Networks based Visual Data Mining for Clinical and Metabolomic Data**; Kasun Amarasinghe¹; Urszula Osinska Warnke²; Naren Gajenthra Kumar¹; Daniel Contaifer¹; Milos Manic¹; Dayanjan S Wijesinghe¹; ¹Virginia Commonwealth University, Richmond, VA; ²Virginia Commonwealth University, Richmond, VA

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- WP 337 **Guiding Ions with a Quadrupole Operated at Elevated Pressure**; Wen-Ping Peng¹; Zhuoer Xie²; Adam Hollerbach²; Dalton T Snyder²; Graham Cooks²; ¹National Dong Hwa University, Shoufeng, Taiwan; ²Purdue University, West Lafayette, IN
- WP 338 **Preclinical Pharmacokinetics Study Using Miniature MS System and Culex Automatic Blood Sampler**; Fan Pu¹; Wenpeng Zhang²; Yong Liu³; Kevin Bateman⁴; Roy Helmy³; Zheng Ouyang^{1,2,5}; ¹Department of Chemistry, Purdue University, West Lafayette, IN; ²Weldon School of Biomedical Engineering, Purdue University, West Lafayette, Indiana; ³Merck Research Laboratories, Rahway, NJ; ⁴Pharmacokinetics, Pharmacodynamics and Drug Metabolism, Merck Research Laboratories, Merck & Co., Inc., West Point, PA; ⁵Department of Precision Instrument, Tsinghua University, Beijing, China
- WP 339 **Comparison of Canine Sniffing Capability with Portable Mass Spectrometry**; Stamatis Giannoukos¹; Boris Brkić¹; Stephen Taylor¹; ¹Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK
- WP 340 **Use of a Hexapole Ion Guide in a Miniature, Low Power LC-MS Interface: The Power vs. Performance Tradeoff**; Adrian Southard¹; Stephanie A Getty²; Jerome P Ferrance³; Jamie E Elsila²; Manuel A Balvin²; Carl A Kotecki²; ¹Universities Space Research Association, Columbia, MD; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³J2F Engineering, Charlottesville, VA
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- van Amerom⁵; Andrej Grubisic⁴; Paul R Mahaffy⁴; William B. Brinkerhoff¹; Graham Cooks¹; ¹Purdue University, West Lafayette, Indiana; ²KapScience LLC, Tewksbury, MA; ³Danell Consulting, Greenville, NC; ⁴NASA GSFC, Greenbelt, MD; ⁵Mini-Mass Consulting, Inc., Hyattsville, MD
- WP 342 **A Miniature Mass Spectrometer with a Miniature Ion Funnel**; Yanbing Zhai¹; Xiaohua Zhang²; Wei Xu¹; ¹Beijing Institute of Technology, Haidian District, Beijing; ²Anyee Instrumentation Company, Suzhou, China
- WP 343 **Optimization of the PerkinElmer Torion T-9 Portable GC/MS for Common Field Analyses**; Joshua Wilhide¹; Ian W Shaffer¹; Margaret E LaCourse¹; William R LaCourse¹; ¹University of Maryland Baltimore County, Baltimore, MD
- WP 344 **Characterization of a Highly Compact Linear Ion Trap Mass Spectrometer (LITMS)**; Friso H.W. Van Amerom¹; Ryan M Danell²; Xiang Li³; Andrej Grubisic⁴; Veronica T. Pinnick⁵; Ricardo D. Arevalo⁵; Stephanie A. Getty⁵; William B. Brinkerhoff⁵; Paul R Mahaffy⁵; ¹Mini-Mass Consulting, Inc, Hyattsville, MD; ²Danell Consulting, Greenville, NC; ³University of Maryland Baltimore County, Baltimore, MD; ⁴University of Maryland, College Park, MD; ⁵NASA GSFC, Greenbelt, MD
- WP 345 **Development of a Portable 13C Isotope Ratio Measurement Technique with Quadrupole Mass Spectrometry**; David McIntosh¹; Stomatis Giannoukos¹; Brian Thomas²; Tom Fildes³; Lynn Smith⁴; Stephen Taylor¹; ¹University of Liverpool, Liverpool, Merseyside; ²University of Liverpool, Glenn Heights, TX; ³University of Liverpool, Liverpool, UK; ⁴Norton Priory, Runcorn, UK

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- WP 347 **Electro-kinetic Assisted Electrospray Ionization for Enhanced Complex Sample Analysis**; Muyi He¹; Zezhen Zhang¹; Pan Luo¹; Jie Hong¹; Wenjing Zhang¹; Jianli Liu¹; Xiaoli Zhang¹; Wei Xu¹; ¹Beijing Institute of Technology, Beijing, Beijing
- WP 348 **Determination of Unbound Urinary Amino Acids Incorporated with Creatinine Normalization by LC-MS/MS Method with CLAM-2000 Online Sample Pre-treatment**; Zhe Sun¹; Jie Xing¹; Irene Agatha²; Daisuke Kawakami³; Zhaoqi Zhan¹; ¹Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd., Singapore, Singapore; ²School of Physical and Mathematical Science, Nanyang Technical University, Singapore, Singapore; ³Clinical & Biotechnology Business Unit, Shimadzu Corporation, Kyoto, Japan
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- Attiki; ³School of Production Engineering & Management, Technical University of Crete, Crete, Greece; ⁴Institute of Microelectronics of Madrid, Tres Cantos, Spain
- WP 352 **Development of a Compact Microwave Driven ICP Atom Source for Hydrogen Attachment/Abstraction Dissociation (HAD) of Tandem Mass Spectrometry;** Yuji Shimabukuro¹; Hidenori Takahashi²; Shinichi Iwamoto²; Koichi Tanaka²; Motoi Wada¹; ¹Doshisha University, Kyotanabe, Japan; ²Shimadzu Corporation, Kyoto
- WP 353 **A Novel Platform of On-line Sample Pre-treatment and LC/MS/MS Analysis for Screening and Quantitation of Illicit Drugs in Urine;** Shao Hua Chia¹; Zhi Wei Edwin Ting¹; Daisuke Kawakami²; Jie Xing¹; Zhaoqi Zhan¹; ¹Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; ²Shimadzu Corporation, Kyoto, Japan
- WP 354 **Gas Assisted Ion Ejection (GAIE) Technique Enables Simultaneous Particle Mass and Size Measurement in a Single Quadrupole Ion Trap Cell;** Caiqiao Xiong¹; Zongxiu Nie¹; ¹Institute of Chemistry, Chinese Academy of Sciences, Beijing, China
- WP 355 **Flavors, Odors, and Contaminants in Alcoholic Beverages using Vacuum Assisted Sorbent Extraction (VASE) and GC/MS Analysis;** Victoria Noad¹; Daniel B. Cardin¹; ¹Entech Instruments, Simi Valley, CA
- WP 356 **Importance of Metal Oxide Dissociation in the Liquid Sampling-Atmospheric Pressure Glow Discharge / Orbitrap System for Isotope Ratio Measurements;** Edward Hoegg¹; Kenneth Marcus¹; ¹Clemson University, Clemson, SC
- WP 357 **A "Brick Ion Trap Mass Spectrometer" Driven by a Frequency Scanning Technique;** Ting Jiang¹; Tang Yang¹; Hongjia Zhang²; Yanbing Zhai¹; Wei Xu¹; Dayu Li²; Wei Xu¹; ¹Beijing Institute of Technology, Haidian District, Beijing; ²Northeastern University, Shenyang, China
- WP 358 **High-Sensitivity and Simultaneous Analysis of Psychoactive Drugs using LC-MS/MS with Full-Automated Pretreatment System;** Daisuke Kawakami¹; Toshikazu Minohata¹; Sihoko Nakano²; Noriaki Shima²; Akihiro Miki²; Munehiro Katagi²; ¹Shimadzu Corporation, Kyoto, Japan; ²Osaka Prefectural Police, Osaka, Japan
- WP 359 **New Digital Mass Scanning Techniques without Dipolar Auxiliary Waveforms;** Katherine G. E. Donahoe¹; Ashley Marie Moon¹; Zachary Philip Gotlib¹; Nathan Michael Hoffman¹; Peter T. A. Reilly²; ¹Washington State University, Pullman, WA; ²Washington State University, Pullman, WA
- WP 360 **Supercritical Fluid Chromatography Coupled to Electron Ionization Mass Spectrometry: Development of a New System;** Francesca Rigano¹; Luigi Mondello^{1,2,3}; ¹Chromaleont s.r.l., Messina, Italy; ²Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Messina, Italy; ³Unit of Food Science and Nutrition, Department of Medicine, University Campus Bio-Medico of Rome, Roma, Italy
- WP 361 **Rapid FAIMS Inside the Mass Spectrometry Envelope: Exploring Ion Mobility Separations in the Extreme-Field Region;** Alexandre Shvartsburg¹; Andrew Entwistle²; Roch Andrzejewski²; Anisha Harris²; Roger Giles²; ¹Wichita State University, Wichita, KS; ²Shimadzu Research Laboratory Europe, Manchester, UK
- WP 362 **On-line Atomic Force Microscope Tip-Enhanced Laser Ablation Mass Spectrometry;** Md Amir Hossen¹; Bijay Banstola¹; Fan Cao¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- WP 363 **Development of Simultaneous, Quantitative Elemental and Molecular Chemical Imaging Via Optical and Mass Spectrometries;** Jake T. Shelley¹; Sunil Badal¹; Montwaun D. Young¹; Brian T. Molnar¹; Courtney L. Walton¹; Garrett M. MacLean¹; ¹Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY
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- WP 366 **Electrospray Ionization Zoom Time-of-Flight Mass Spectrometry;** Christopher Brails¹; Jonas Metternich²; Steven Ray¹; ¹University at Buffalo, Buffalo, NY; ²University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany

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- WP 368 **Screening of Human Fetal Hippocampus Gangliosides by Ion Mobility Mass Spectrometry;** Mirela Sarbu^{1,2}; Željka Vukelić³; David E Clemmer⁴; Alina D Zamfir^{1,2}; ¹National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; ²"Aurel Vlaicu" University of Arad, Arad, Romania; ³Department of Chemistry and Biochemistry, University of Zagreb Medical School, Zagreb, Croatia; ⁴Indiana University, Bloomington, IN
- WP 369 **Separation of Isomeric Sphingosines using Trapped Ion Mobility QTOF-MS;** Matt Willetts¹; Dirk Wunderlich²; Verena Tellstroem²; ¹Bruker Daltonics, Billerica, MA; ²Bruker Daltonik GmbH, Bremen, Germany
- WP 370 **Improved Metabolomics Analysis using Isotopic Ratio Outlier Analysis (IROA) with Ion Mobility-Mass Spectrometry;** Robin H.J. Kemperman¹; Chris W.W. Beecher^{1,2}; Richard A. Yost¹; ¹University of Florida, Gainesville, FL; ²IROA Technologies, Gainesville, FL
- WP 371 **Improved Sensitivity for Shotgun Proteomics on a Novel Trapped Ion Mobility Spectrometry (TIMS) – Quadrupole Time-of-Flight (QTOF) Instrument;** Scarlet Beck¹; Heiner Koch¹; Florian Meier¹; Markus Lubeck²; Stephanie Kaspar-Schoenefeld²; Niels Goedecke²; Oliver Raether²; Juergen Cox¹; Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Bruker Daltonik GmbH, Bremen, Germany
- WP 372 **Optimizing Sample Introduction for Quantitation of 25-Hydroxyvitamin D in Human Serum using Liquid Chromatography/Ion Mobility/Mass Spectrometry;** Jiajun Lei¹; Nicholas R. Oranzi¹; Richard A. Yost¹; ¹University of Florida, Gainesville, FL
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- WP 374 **High Resolution Trapped Ion Mobility Mass Spectrometry Analysis of Pharmaceutical Intermediate products;** Qinghe Wang¹; Keyu Zhou¹; Jing Lu²; Kefei Wang¹; ¹Bruker Daltonics, Shanghai, China; ²Bruker Daltonics, Beijing, China
- WP 375 **Evaluation of the Precision of Ion Mobility Mass Spectrometry for Coulombic Unfolding of Intact Proteins and Disulfide Bond Characterization;** David McCaskill¹; John Patrick O'Brien²; Krishna Kuppannan¹; Jeffrey Gilbert¹; Ruwan Kurulugama³; Garrison Birch³; John Fjeldsted³; ¹Dow AgroSciences, Indianapolis, IN; ²The Dow Chemical Company, Midland, MI; ³Agilent Technologies Inc., Santa Clara, CA



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- WP 377 **Drug-Protein Interaction and Biomolecular Conformation Analysis by High-Resolution Ion Mobility-Mass Spectrometry**; [Urs Rohner](#)¹; Matthew P. Sullivan²; David C. Goldstone³; Christian G. Hartinger²; Michael Groessl⁴; ¹TOFWERK, Thun, Switzerland; ²School of Chemical Sciences, University of Auckland, Auckland, New Zealand; ³School of Biological Sciences, University of Auckland, Auckland, New Zealand; ⁴Department of Clinical Research, Bern, Switzerland
- WP 378 **Rapid Differentiation of Chemically Modified Insulin Isomers by Ion Mobility – Mass Spectrometry**; [Weijuan Tang](#)¹; Nicholas Pierson¹; Gregory Pirrone¹; Alexey Makarov¹; Shane Krska²; ¹Analytical Research & Development, Merck & Co. Inc., Rahway, NJ; ²Discovery Chemistry, Merck & Co., Inc., Kenilworth, NJ
- WP 379 **Rapid Monitoring of Glutathione-Adduction Reactions by Ion Mobility-Mass Spectrometry**; [Dylan Ross](#)¹; Kelly M. Hines¹; Michele Scian¹; Libin Xu¹; ¹Department of Medicinal Chemistry, University of Washington, Seattle, WA
- WP 380 **Structural Characterization of PEGylated Proteins via Ion Mobility Mass Spectrometry**; [John P O'Brien](#)¹; Kevin P O'Donnell¹; David M Meunier¹; ¹Dow Chemical Company, Midland, MI
- WP 381 **Ion Mobility Mass Spectrometry Reveals Details of Formation and Structure for DNA Triplexes**; [Tara Pukala](#)¹; Alexander Begbie¹; Jiawei Li¹; David Huang¹; ¹University of Adelaide, Adelaide, South Australia
- WP 382 **Characterization of N-linked Isomeric Glycans Using LC and Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) with Mass Spectrometry**; [Daniel Delafield](#)¹; Zhe Wang¹; Matthew Baird²; Alexandre A. Shvartsburg³; Si Wu¹; Kenneth Smith⁴; ¹University of Oklahoma, Norman, OK; ²Wichita State University, Wichita, KS - Kansas; ³Wichita State University, Wichita, KS; ⁴Oklahoma Medical Research Foundation, Oklahoma City, OK
- WP 383 **Anion Attachment for Separation of Isomeric Steroids by Trapping Ion Mobility Spectrometry (TIMS) - ToF**; [Richard B. Cole](#)¹; Christian Albers²; Dorith Brombach²; ¹Sorbonne Universités - UPMC (Paris 6), Paris, France; ²Brüker Daltonik GmbH, Bremen, Germany
- WP 384 **On the Accuracy of Poly-DL-Alanine Calibration in T-Wave Ion Mobility**; [Bela Paizs](#)^{1,2}; Daniel Chaplin¹; Keith Richardson³; Nick Tomczyk³; Kevin Giles³; Zoltan Takats^{2,4}; ¹Bangor University, Bangor, Gwynedd; ²deShape Ltd., Bangor, UK; ³Waters Corporation, Wilmslow, UK; ⁴Imperial College London, London, England
- WP 385 **Structural Characterization of HMGA2 and HMGA2-DNA complexes using nanoESI-CIA-HDX-TIMS-MS**; [Alyssa L. Garabedian](#)¹; Alexander Bolufer¹; Prem Chapagain¹; Fenfei Leng^{1,2}; Francisco A. Fernandez Lima^{1,2}; ¹Florida International University, Miami, FL; ²Biomolecular Sciences Institute, Miami, FL
- WP 386 **Structural Characterization of Multi-Stranded DNA Topologies using nanoESI-CIA-TIMS-MS**; [Jacob Porter](#)¹; Alyssa L. Garabedian¹; Francisco Fernandez Lima^{1,2}; ¹Florida International University, Miami, FL; ²Biomolecular Sciences Institute, Miami, FL
- WP 387 **Time-resolved Ion Mobility-Mass Spectrometry Reveals Structural Transitions in the Disassembly of Modular Polyketide Synthases**; [Chunyi Zhao](#)¹; Joseph D. Eschweiler¹; Samuel T. Slocum²; David H. Sherman^{1,2}; Brandon T. Ruotolo¹; ¹University of Michigan Chemistry

Department, Ann Arbor, MI; ²University of Michigan Life Sciences Institute, Ann Arbor, MI

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- WP 467 **Untargeted Discovery SWATH vs Targeted dynamic MRM Analysis for Quantitative Metabolomics Profiling of a Mutant Melanoma Line;** Li Zhang¹; Lauren Rodenbarger²; Daniel Kremer³; Maureen Kachman⁴; David Lombard²; Costas Lyssiotis³; ¹The Michigan Regional Comprehensive Metabolomics Research Core, University of Michigan, Ann Arbor, MI; ²Department of Pathology, University of Michigan, Ann Arbor, MI; ³Department of Molecular and Integrative Physiology, University of Michigan, Ann Arbor, MI; ⁴Michigan Regional Comprehensive Metabolomics Resource Center, University of Michigan, Ann Arbor, MI
- WP 468 **Comparative Metabolomics Study Revealing Staphylococcus Aureus Metabolic Response to Different Antibiotics;** Jiangjiang Zhu; Miami University, Oxford, OH
- WP 469 **Metabolic Determination of Acetaminophen in Down Syndrome Disease Research Using Targeted Mass Spectrometry;** Melanie Juba¹; Christina Iverson²; Olivia Iverson³; Jeffery Miller¹; Baljit Ubhi¹; ¹SCIEX, Redwood City, CA; ²Algonquin Regional High School, Northborough, MA; ³Boston University, Boston, MA
- WP 470 **Simultaneous and Comprehensive Determination of Tryptophan and its Catabolites in Mouse Tissues by Polarity Switching UHPLC-MRM-MS;** Guan-yuan Chen¹; Wei Zhong¹; Zhanxiang Zhou^{1,2}; Qibin Zhang^{1,3}; ¹Center for Translational Biomedical Research, University of North Carolina at Greensboro, Kannapolis, NC; ²Department of Nutrition, University of North Carolina at Greensboro, Greensboro, NC; ³Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC
- WP 471 **A Novel GC-MS Assay for Quantitation of Short Chain Fatty Acids in Human Plasma;** Linxing Yao¹; Emily A. Davidson¹; Corey D. Broeckling¹; Jessica E. Prenni¹; ¹Proteomics and Metabolomics Facility, Colorado State University, Fort Collins, CO
- WP 472 **LC-MS-Based Metabolomics Revealed SLC25A22 as an Essential Regulator in the Aspartate-Derived Amino Acids and Polyamines in KRAS-Mutant Colorectal Cancer;** Xiaona Li¹; Chi Chun Wong²; Zongwei Cai^{1*}; ¹State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; ²Institute of Digestive Disease and Department of Medicine and Therapeutics, State Key Laboratory of Digestive Disease, Li Ka Shing Institute of Health Sciences, Chinese University of Hong Kong, Hong Kong, China
- WP 473 **Towards Quantification of Anti-Cancer Compounds in Individual Patient Bladder Cancer Cells;** Shawna Standke¹; Ning Pan¹; Naga Rama Kothapalli¹; Anh T. Le¹; C. A. Malinky²; Anthony W. Burgett¹; Zhibo Yang¹; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Norman, OK
- WP 474 **Quantification of polyamines and Urea Cycle Metabolites in Biological Samples by HILIC-MS;** Judy Baek¹; Stefanie Wernisch¹; Yun Jin Sin²; Jaeman Byun¹; Subramaniam Pennathur¹; ¹University of Michigan Medical Center, Ann Arbor, MI; ²University of Michigan, Ann Arbor, MI
- WP 475 **Effect of Stress on Eucalyptus Plant Metabolome;** Seetaramanjaneyulu Gundimeda¹; Daniela Feltrim²; Paulo Mazzafera²; ¹Agilent technologies, Bangalore, India; ²Plant Biology Department, State University of Campinas, Campinas, Brazil
- WP 476 **Enhanced Targeted Metabolomics with High Resolution MS – Adaption of a Standardized Metabolomics Assay from Triple Quad to Orbitrap MS;** Hai Pham Tuan¹; Doreen Kirchberg¹; Martin Buratti¹; Simon Schafferer¹; Kristaps Klavins¹; Glenn Damkroeger²; Madalina Oppermann²; Anastasia Kalli³; Reiko Kiyonami³; David Peake³; Andreas Huhmer³; Therese Koal¹; ¹BIOCRATES Life Sciences AG, Innsbruck, Tyrol; ²Thermo Fisher Scientific, Bremen, Germany; ³Thermo Fisher Scientific, San Jose, CA
- WP 477 **Determination of 8-oxo-7,8-dihydroguanosine in Urine from Patients with Colorectal Cancer using Ultra Performance Liquid Chromatography–Tandem Mass Spectrometry;** Cheng Guo¹; Shu Zheng¹; ¹Zhejiang University, Hangzhou, Zhejiang
- WP 478 **NMR Guided Mass Spectrometry for Absolute Quantitation of Human Blood Metabolites;** Daniel Raftery¹; G. A. Nagana Gowda¹; Danijel Djukovic¹; Haiwei Gu¹; ¹UW Medicine, SLU, Seattle, WA
- WP 479 **Identification of Race-Associated Metabolite Biomarkers for Hepatocellular Carcinoma;** Cristina Di Poto¹; Shisi He¹; Rency S. Varghese¹; Yi Zhao²; Alessia Ferrarini¹; Abdullah Karabala³; Habtom W. Resson¹; ¹Georgetown University, Lombardi Cancer Center, Washington, DC; ²Brown University, Providence, RI; ³MedStar Georgetown University Hospital, Washington, DC
- WP 480 **Racial Disparity in Bladder Cancer and Identification of Altered Metabolism in African American Compared to European Bladder Cancer;** Sri Ramya Donepudi¹; Venkatrao Vantaku¹; Tiffany Dorsey²; Vasanta Putluri³; Suman Maity³; Wei Tang²; Feng Jin³; Danthasinghe Waduge Badrajee Piyaarathna³; Kimal Rajapakshe³; MeghaShyam Kavuri³; Vadiraja Bhat⁴; Seth Lerner³; Yair Lotan⁵; Wei Liu⁶; Cristian Coarfa³; Arun Sreekumar³; Stephan Ambs²; Nagireddy Putluri³; ¹Baylor College of Medicine, Houston, TX; ²NIH, Bethesda, MD; ³Baylor College of Medicine, Houston, TX; ⁴Agilent Technologies Inc., Santa Clara, California; ⁵UT Southwestern, Dallas, TX; ⁶Agios Pharmaceuticals, Boston, MA



- WP 481 **Mass Spectrometry Analysis of Omega-3 PUFA in RBC, PBMCs, DBS and their Anti-Inflammatory Metabolite;** Boakye Gyimah¹; Martin R Lindley¹; Mark Platt¹; James Reynolds¹; ¹Loughborough University, Loughborough
- WP 482 **Tobacco-specific Carcinogens Induce Hypermethylation, DNA Adducts and DNA Damage in Bladder Cancer;** Feng Jin¹; Jose Thaiparambil²; Sri Ramya Donepudi¹; Vasanta Putluri¹; Vadiraja Bhat³; Preeti Purwaha¹; Danthasinghe Waduge Badrajee Piyarathna¹; Rashmi Krishnapuram¹; Franklin Gu¹; Suman Maity¹; Salil Kumar¹; Chandra Shekar R Ambati¹; Friedrich-Carl von Rundstedt¹; Daniel Godde¹; Stephan Roth¹; Stephan Storkel¹; George Michailidis¹; Balasubramanyam Karanam¹; Martha Terris¹; Shyam Kavuri¹; Seth Lerner¹; Cristian Coarfa¹; Yair Lotan¹; Arun Sreekumar¹; Nagireddy Putluri⁴; ¹Baylor College of Medicine, Houston, TX; ²Houston Methodist Research Institute, Houston, TX; ³Agilent Technologies, Inc., Wilmington, DE; ⁴Baylor College of Medicine, Houston, TX
- WP 483 **Simultaneous Determination of Key Glycolysis and Tricarboxylic Acid Cycle Intermediates in Fluxomics Studies by DMS-LC/MS/MS;** Mary A Piotrowski¹; Darren Dumlaio¹; Julie Keefer¹; John Janiszewski¹; Richard Kirkbey²; Tiago Alves²; Bradley B Schneider³; Chang Liu³; J. Larry Campbell³; Paul RS Baker³; Yves LeBlanc³; Keith J. Goodman³; Tanya Gamble³; ¹Pfizer Inc., Groton, CT; ²Yale University, New Haven, CT; ³Sciex, Concord, ON, Canada

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- WP 485 **Distinct Proteome Remodeling of Industrial Saccharomyces Cerevisiae in Response to Prolonged Thermal Stress or Transient Heat Shock;** Weidi Xiao¹; Xiaoxiao Duan¹; Yuping Lin²; Qinchao Cao²; Qinhong Wang²; Wengqing Shui^{2,3}; ¹College of Life Sciences, Nankai University, Tianjin, China; ²Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, Tianjin; ³Human Institute, ShanghaiTech University, Shanghai, China
- WP 486 **Development of an Automated Mass Spectrometry-based System to Study Dynamics of Microbial Volatomes;** Cheng Hao Chang¹; Pawel L. Urban¹; ¹National Chiao Tung University, Hsinchu, Taiwan
- WP 487 **Oral Microbiota in Down Syndrome Individuals: Identification by MALDI-Biotyper;** Rafael Celestino Souza^{1,2}; Levy Anderson Alves^{1,3,4}; Meriellen Dias^{2,4}; Fausto Medeiros Mendes¹; Ana Lidia Ciamponi¹; Maria Anita Mendes^{2,4}; ¹Dental School of USP, São Paulo, Brazil; ²Universidade de São Paulo - USP, São Paulo, South America; ³Guarulhos University, Guarulhos, Brazil; ⁴Dempster Mass Lab- POLI- USP, São Paulo, Brazil
- WP 488 **Identification of ESKAPE Pathogens by MALDI-TOF MS Analysis of Microbial Membrane Glycolipids;** Lisa Leung¹; William E Fondrie¹; Yohei Doi²; J Kristie Johnson¹; Dudley K Strickland¹; Robert K Ernst¹; David R Goodlett¹; ¹University of Maryland, Baltimore, Maryland; ²University Of Pittsburgh, Pittsburgh, PA
- WP 489 **Proteomic Comparisons Between Aspergillus fumigatus Isolates from the International Space Station and Terrestrial Reference Strains;** Abby J Chiang¹; Adriana Blachowicz^{2,3}; Clay C.C. Wang^{3,4}; Teresa B. Hong¹; Kasthuri Venkateswaran²; Markus Kalkum¹; ¹Beckman Research Institute of City of Hope, Duarte, CA; ²Biotechnology and Planetary Protection Group, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; ³Department of Pharmacology and Pharmaceutical Sciences, School of Pharmacy, University of Southern California, Los Angeles, CA; ⁴Department of Chemistry, Dornsife College of Letters, Arts and Sciences, University of Southern California, Los Angeles, CA
- WP 490 **Qualitative and Quantitative Analysis of Hemolytic Toxins from Dinoflagellates Specifically Associated with Fish Kills by Mass Spectrometry;** Benjamin L. Oyler^{1,2}; Saddef Haq^{1,2}; David R. Goodlett³; Allen R. Place²; ¹University of Maryland School of Medicine, Baltimore, MD; ²Institute of Marine and Environmental Technology, University of Maryland Center for Environmental Science, Baltimore, MD; ³University of Maryland School of Pharmacy, Baltimore, MD
- WP 491 **Ultra-Rapid Identification of Bacteria by MALDI-TOF MS;** Tao Liang¹; Young In Lee²; Lisa M Leung^{1,2}; SUNG HWAN Yoon²; Alison J Scott²; Robert K Ernst²; David R Goodlett¹; ¹Department of Pharmaceutical Science, School of Pharmacy, University of Maryland, Baltimore, Baltimore, MD; ²Department of Microbial Pathogenesis, School of Dentistry, University of Maryland, Baltimore, MD
- WP 492 **MycDB: New Spectral Database for Identification of Mycobacterium species by MALDI-TOF MS;** Kyu H. Park¹; Jae-Seok Kim²; Sue Shin³; Taek Soo Kim³; Eun-Kyeong Choi¹; Yongha In¹; Hyung Soon Park¹; Yongsun Kim¹; ¹ASTA, Suwon, South Korea; ²Department of Laboratory Medicine, Hallym University College of Medicine, Chuncheon, South Korea; ³Seoul National University College of Medicine, Jongno-gu, South Korea
- WP 493 **Fast Detection of Carbenicemase-Producing Acinetobacter baumannii using Nanodiamonds and MALDI-TOF MS;** Kai-Chih Chang¹; Chin-Yi Chung²; Chen-Hsing Yeh¹; Kuo-Hsiu Hsu²; Hsi-An Chen²; Ya-Chin Chin²; Anren Hu¹; Po-Chi Soo¹; Wen-Ping Peng²; ¹Tzu Chi University, Hualien, Taiwan; ²National Dong Hwa University, Shoufeng, Taiwan
- WP 494 **Proteogenomic Characterization of Escherichia coli ATCC8739 used for MALDI-TOF Calibration in VITEK-MS;** Frédéric Jaufrut^{1,2}; Corinne Beaulieu¹; Jean-Pierre Cotte-Pattat³; Victoria Girard³; Martin Welker³; Céline Brochier-Armanet²; Jean-Pierre Flandrois²; Jean-Philippe Charrier¹; ¹biomerieux, Marcy L'etoile, Rhone-Alpes; ²Université Claude Bernard Lyon-1, Villeurbanne, France; ³Biomerieux, La Balme Les-Grottes, France
- WP 495 **Profiling of Small Molecules for the Discrimination of Bacillus cereus and Bacillus thuringiensis by MALDI-TOF MS ;** Yongsun Kim¹; Miyoung Ha²; Eun-Kyeong Choi³; Yongha In³; ¹ASTA, Suwon, Gyeonggi; ²Nonghyup Food Research Institute, Suwon-si, South Korea; ³ASTA, Suwon, South Korea
- WP 496 **Proteomic Characterization of Particle Content and Infectious Cycle of Pandoraviruses, A Recently Discovered Family of Giant Viruses.;** Laure Beucher¹; Elisabeth Fabre²; Lucid Blumdes¹; Matthieu Legendre²; Anne-Marie Hesse¹; Olivier Poirot²; Sandra Jeudy²; Christophe Bruley¹; Jean-Michel Claverie²; Chantal Abergel²; Yohann Couté¹; ¹EDyP UMR1038 Inserm/CEA/UGA, Grenoble, France; ²Information Génomique & Structurale, Unité Mixte de Recherche 7256 (Institut de Microbiologie de la Méditerranée, FR3479) Centre National de la Recherche Scientifique, Marseille cedex 9, France
- WP 497 **Identification of Common Food-Borne Pathogens at Species and Sub-Species Level by LC-MS/MS;** Shu-Hua Chen¹; Christine H. Parker¹; Timothy R. Croley¹; Melinda A. McFarland¹; ¹U.S. Food and Drug Administration, College Park, MD



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- WP 498 **Recognition of Clostridium difficile PCR-Ribotypes by Intact Protein Analysis Using Ultrahigh Resolution MALDI-FTICR MS**; Simone Nicolardi¹; Jeff A. Sen¹; Bart Mertens¹; Ingrid M.J.G. Sanders¹; Paul J. Hensbergen¹; Ed J. Kuijper¹; ¹Leiden University Medical Center, Leiden, Netherlands
- WP 499 **Nicotine-Induced Proteome of Arthrobacter nicotinovorans pAO1+**; Marius Mihasan^{1,2}; Cornelia Babii¹; Roshanak Aslebagh²; Costel C. Darie²; ¹Biochemistry and Molecular Biology Laboratory, Faculty of Biology, Alexandru Ioan Cuza University, Iasi, Romania; ²Biochemistry & Proteomics Group, Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY
- WP 500 **Quantitative Proteome Analyses of Diverse Mycobacterium Tuberculosis Clinical Isolate Strains by SWATH-MS**; Ben Collins¹; Amir Banaei-Esfahani^{1,2}; Olga T. Schubert^{1,3}; Andrej Trauner⁴; Sonia Borrell⁴; Mireia Coscolla⁴; Sebastien Gagneux⁴; Ruedi Aebersold^{1,5}; ¹Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; ²PhD Program in Systems Biology, University of Zurich and ETH Zurich, Zurich, Switzerland; ³Present address: Departments of Human Genetics, University of California, Los Angeles, CA; ⁴Department of Medical Parasitology and Infection Biology, Swiss Tropical and Public Health Institute, Basel, Switzerland; ⁵Faculty of Science, University of Zurich, Zurich, Switzerland
- WP 501 **Mass Spectrometry Imaging and Electron Microscopy of Drip-Flow Generated Biofilm Induced Corrosion**; Joseph F. Ellis¹; Bin Li¹; Sage J. B. Dunham¹; Justin D. Lange²; Clint M. Arnett²; Jonathan V. Sweedler¹; ¹Department of Chemistry and the Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL; ²Engineer Research and Development Center-Construction Engineering Research Laboratory (ERDC-CERL), Champaign, IL
- WP 502 **Metabolite Monitoring of Pseudomonas aeruginosa using Rapid Evaporative Ionization Mass Spectrometry and Applications for Strain Typing and Infection Diagnosis**; Emmanuelle E. Bardin¹; Simon J.S. Cameron¹; Alvaro Perdones-Montero¹; Kate Hardiman¹; Eric W.F.W. Alton¹; Andrew Bush^{1,2}; Jane C. Davies^{1,2}; Zoltan Takats¹; ¹Imperial College London, London, London; ²Royal Brompton and Harefield NHS Foundation Trust, London, UK
- WP 503 **Stable Isotope Labeling of Borrelia burgdorferi (SILAB): Quantitative Proteomic Analysis of the Agent of Lyme Disease**; Susan T. Weintraub¹; Trevor C. Smith, Jr.²; Sarah M. Helm²; Sammy Pardo¹; Dana Molleur²; J. Seshu²; ¹UT Health San Antonio, San Antonio, TX; ²University of Texas at San Antonio, San Antonio, TX
- WP 504 **Detection and Subtyping of Shiga Toxins (Stx) from Escherichia Coli Culture using Parallel Reaction Monitoring**; Leanne Scharikow^{1,2}; Stuart McCorrister¹; Derek Davlut¹; Patrick Chong¹; Morag Graham^{1,2}; Garrett Westmacott¹; ¹Public Health Agency Canada, Winnipeg, MB; ²University of Manitoba, Winnipeg, MB
- WP 505 **pMSGF+: A Two-Stage Database Search Approach Improving Speed and Sensitivity for Metaproteomics Studies**; Miin S. Lin¹; Doruk Beyter¹; Vineet Bafna¹; ¹University of California, San Diego, La Jolla, CA
- WP 506 **LC-MS Analysis of Extracellular Proteins for the differentiation of Bacillus cereus and Bacillus thuringiensis**; Jennifer Brzezinski¹; Geoffrey Kilili¹; Kirk Gaston¹; ¹FDA, Forensic Chemistry Center, Cincinnati, OH
- WP 507 **Are Cysteine and Methionine Synthesis Proteins Essential for Dormancy in Actinobacteria?**; Morgan Mitchell¹; Sujina Mali¹; Spencer Havis¹; Abiodun Bodunrin¹; Jonathan Rangel¹; Steven Bark¹; William Widger¹; ¹University of Houston, Houston, TX
- WP 508 **A Proteomic Signature of Dormancy in an Actinobacterium: Micrococcus luteus**; Sujina Mali¹; Morgan Mitchell¹; Spencer Havis¹; Abiodun Bodunrin¹; Jonathan Rangel¹; William R. Widger¹; Steven J. Bark¹; ¹University of Houston, Houston, TX
- WP 509 **Rapid Characterization of Microbial Samples via Extractive Sampling and Ionization**; Mariam S. Elnaggar; Prosolia, Inc., Indianapolis, IN
- WP 510 **Possible Ribosomal Regulation in the Viable but Non-Culturable State of Micrococcus luteus**; Spencer Havis¹; Sujina Mali¹; Morgan Mitchell¹; Abiodun Bodunrin¹; Jonathan Rangel¹; William Widger¹; Steven Bark¹; ¹University of Houston, Houston, TX
- WP 511 **Use of Mass Spectrometry in the Hunt for Novel Lytic Bacteriophage Active Against Pathogenic E. coli.**; Leslie Harden¹; Yen-Te Liao¹; Anna Bates¹; Vivian Wu¹; ¹USDA/WRRC, Albany, CA
- WP 512 **Meta-Proteomics Analysis of a Biofilm Community Reveals Synergistic Interactions in a Microbial Consortium**; Zacharias Brimnes Visby Damholt¹; Jakob Herschend²; Andrea Marion Marquard¹; Birte Svensson¹; Søren J. Sørensen²; Per Hågglund¹; Mette Burmølle²; ¹Technical University of Denmark, Lyngby, Denmark; ²University of Copenhagen, Copenhagen, Denmark
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- WP 514 **Characterization of Polystyrene and Silica Beads in Submicrometer Range using Flow Filed-Flow Fractionation and Flow Cytometry**; Zhishang Hu¹; Chen Ye²; Wei Mi³; Hongmei Li³; Haiying Hang²; ¹NIM, China, Beijing, Beijing; ²IBP, CAS, China, Beijing, China; ³NIM, China, Beijing, China
- WP 515 **A Sensitive Microflow LC/MS/MS Method for the Analysis of Fluticasone Propionate in Human Plasma**; Angela Doneanu¹; Michael Donegan¹; James Murphy¹; ¹Waters Corporation, Milford, MA
- WP 516 **Novel Aspects and Performance Evaluation of a Liquid-El LC-MS Interface**; Maurizio Piergiovanni¹; Giorgio Famiglini¹; Pierangela Palma¹; Veronica Termopoli¹; Achille Cappiello¹; ¹University of Urbino, Urbino
- WP 517 **Dynamic pH Junction Based Capillary Zone Electrophoresis-Mass Spectrometry with Half-a-Microliter Loading Capacity and 140-min Separation Window for Bottom-Up Proteomics**; Daoyang Chen¹; Liangliang Sun¹; Xiaojing Shen¹; ¹Michigan State University, East Lansing, MI
- WP 518 **Fast Chip-CEMS for Characterization of Protein/PTM Changes**; Deborah R. Leon¹; Kshitij Khatri¹; Bo Yan¹; John R. Hasserick¹; Christian Heckendorf¹; Joseph Zaia¹; Catherine E. Costello¹; Mark E. Mccomb¹; ¹Boston University School of Medicine, Boston, MA
- WP 519 **Capillary Electrophoresis and Ion Mobility Coupled to Mass Spectrometry as Complementary Tools for Cysteine Connectivity Identification in Peptides**; Cedric Delvaux¹; Philippe Massonnet¹; Christopher Kune¹; Jean R. N. Haler¹; Grégory Upert²; Gilles Mourier²; Nicolas Gilles²; Loïc Quinton¹; Johann Far¹; Edwin De Pauw¹; ¹Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; ²Commissariat à l'Energie Atomique et aux Energies Alternatives, iBiTec-S, SPI, LEMM, Gif Sur Yvette, France
- WP 520 **Characterization of Anions by Microchip Capillary Electrophoresis-Negative Electrospray Ionization-Mass Spectrometry**; Justin M. Godinho¹; J. Michael Ramsey¹; ¹The University of North Carolina at Chapel Hill, Chapel Hill, NC



WP 521 **A Fully Automated Microchip Capillary Electrophoresis-ESI-MS System for High Throughput Analysis of Metabolites, Peptides, and Intact Proteins**; Joshua P. Guerrette¹; Erin A. Redman¹; Michael P. Goodwin²; J. Scott Mellors¹; ¹908 Devices, Inc., Carrboro, NC; ²908 Devices Inc., Boston, MA

WP 522 **Ionic Liquid-Based Slug-Flow Microextraction for Ambient Ionization Mass Spectrometry**; Yueguang Lv^{1,2}; Qiang Ma¹; ¹Chinese Academy of Inspection and Quarantine, Beijing, China; ²University of Chinese Academy of Sciences, Beijing, China

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WP 524 **Natural Product Bioactive Peptide Discovery using PepSAVI-MS**; Christine L. Kirkpatrick¹; Nicole C. Parsley²; Leslie M. Hicks²; ¹, Chapel Hill, NC; ²UNC-Chapel Hill, Chapel Hill, NC

WP 525 **Valve Based 2D-UHPLC/QTOF MS Solution for Exploring Natural Products**; Guoqiang Liu¹; Yue Song¹; Bo Chen¹; Shan-An Chan²; ¹Agilent Technology, Shanghai, China; ²Agilent Technology, Taipei, Taiwan

WP 526 **MagMASS as a Drug Discovery Platform - Screening Actinobacteria for Novel Ligands of Fructose-1,6-Bisphosphatase**; Michael D. Rush¹; Brian T. Murphy¹; Richard B. van Breemen¹; ¹University of Illinois at Chicago College of Pharmacy, Chicago, IL

WP 527 **Quantification of Aconite Alkaloids in Chinese Proprietary Medicines by LC-ESI-MS/MS and its Application in Product Safety Evaluation**; Ge Xiaowei¹; Yun Zeng¹; Chee-Leong Kee¹; Min-Yong Low¹; ¹Health Sciences Authority, Singapore, Singapore

WP 528 **MS-based Screening of Licorice Extracts for Chemopreventive Agents that Covalently Modify Keap1 Protein, A Regulator of the Antioxidant Response element**; Lingyi Huang¹; Amanda E. Lee¹; Charlotte Simmler¹; Yang Yu¹; Shao-Nong Chen¹; Guido F. Pauli¹; Richard B. van Breemen¹; ¹University of Illinois at Chicago College of Pharmacy, Chicago, IL

WP 529 **Characterization of the Secondary Metabolome of Penicillium using Isotopic Labeling and HPLC-HRMS**; Thaïs Hautbergue^{1,2}; Olivier Puel¹; Souria Tadrist¹; Laurent Debrauwer^{1,2}; Isabelle P. Oswald¹; Emilien L. Jamin^{1,2}; ¹Toxalim (Research Centre in Food Toxicology), Toulouse University, INRA, ENVT, INP-Purpan, UPS, Toulouse, France; ²INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France

WP 530 **Rapid Glucosinolate Detection and Identification using Accurate Mass MS-MS**; Mark Berhow; USDA, ARS, NCAUR, Peoria, IL

WP 531 **Qualitative and Quantitative Determination of Cannabinoid Profiles and Potency in Hemp Oil using LC-UV-MS**; Mike Adams¹; Annette Roth¹; Sue D'Antonio²; Guannan Li²; John Palmer²; Jamie Dougherty²; Anthony Macherone^{2,3}; ¹CWC Labs, Austin, TX; ²Agilent Technologies Inc., Santa Clara, CA; ³Johns Hopkins University School of Medicine, Baltimore, MD

WP 532 **Metabolite Profiling and Localization of Triterpene Glycosides from the Sea Cucumber Eupentacta Fraudatrix**; Roman S. Popov¹; Pavel S. Dmitrenok¹; ¹G.B. Elyakov Pacific Institute of Bioorganic Chemistry,

Far Eastern Branch of the Russian Academy of Sciences, Vladivostok, Russia

WP 533 **Tracking the Bryostatin β -branching Type II Polyketide Synthase "In-action" via Optimized Digestion and nLC-FTMS**; Phillip J. McClory¹; Samuel T. Slocum²; Vikram V. Shende¹; David H. Sherman¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan Medical School, Ann Arbor, MI

WP 534 **Using Multiple Complimentary Analytical Platforms to Investigate Synergistic Relationships between Bioactive Compounds in Natural Herbal Extracts**; Phillip Kirkland¹; Alex Yiannikouris¹; ¹Alltech, Inc., Nicholasville, KY

WP 535 **Identification of the Surface Abiotic Degradation Products of UK-2A and the Biological Activity Relevance**; Quanbo Xiong¹; Kyung Myung²; Chenglin Yao²; Paul R. Graupner²; Yelena Adelfinskaya²; John F. Daeuble²; Meyer T. Stacy²; Zachary Buchan²; Nick X. Wang²; Kevin G. Meyer²; ¹Dow AgroSciences, Indianapolis, IN; ²Dow AgroSciences, Indianapolis, IN

WP 536 **Approaches to Monitor Reactions of Small Molecules with Cell Membranes and Peptides with Cell Membranes by Liquid Chromatography-Mass Spectrometry**; Hannah M Britt¹; Vian S. Ismail¹; John M. Sanderson¹; Jackie Mosely¹; ¹Department of Chemistry, Durham University, Durham, UK

WP 537 **Discovering Metabolites Using Molecular networking: Case Studies for Biomarker Discovery from Cystic Fibrosis Sputa and Patient Metabolism of Antihypertensive Drugs**; Natalie Castellana¹; Anand Patel¹; ¹Digital Proteomics, LLC., La Jolla, CA

WP 538 **Characterization of Polyphenol Derivatives in Pinus Armandii Franchet by Solvent-Compensation Liquid Chromatography Applied with Energy-Resolved Mass Spectrometry**; Pai-Chi Syue¹; Ya-Zhu Zhang¹; Mai-Su Lin¹; Kuo-Lung Ku¹; ¹National Chiayi University, Chiayi City, Taiwan

WP 539 **The Features of the Fragmentations of Rare Starfish Cyclic Steroidal Glycosides in the ESI MS/MS Spectra**; Pavel Dmitrenok; G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Far Eastern Branch of the Russian Academy of Sciences, Vladivostok, Russia

WP 540 **A Rapid Method for Evaluation the Quality of Tea through Screening the Secondary Metabolites by Screen-Printed Carbon Electrode Spray**; Che-I Liao¹; Zong-Yi Wu¹; Kuo-Lung Ku¹; ¹National Chiayi University, Chiayi City, Taiwan

WP 541 **A Tale of Two Cultures: Co-culturing of a Fungus with MRSA**; Diana Kao¹; Huzefa A. Raja¹; Daniel A. Todd¹; Nadja B. Cech¹; Nicholas H. Oberlies¹; ¹University of North Carolina at Greensboro, Greensboro, NC

WP 542 **Cordyceps: A Biologically Complex Age-Old Fungal Medicine**; Chad C. Nelson¹; Krishna Parsawar²; Douglas N. Stevenson¹; ¹Nu Skin Enterprises, Provo, UT; ²University of Utah, Salt Lake City, UT

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WP 544 **Probing the Stoichiometry and Binding Interfaces of Retroviral RNA-Peptide Complexes by Native Top-Down Mass Spectrometry**; Eva-Maria Schneeberger¹; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Tirol

WP 545 **HRAM-LC/MS3 DNA Adductomic Approach, A Comprehensive Methodology to Investigate DNA Damage Induced by Nanomaterials**; Andrea Carra¹; Silvia Balbo¹; Tian Qiu²; Peter W. Villalta¹; Taylor Linn³; Vivian



- Feng³; Christy Haynes²; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²University of Minnesota Twin Cities, Chemistry Department, Minneapolis, MN; ³Augsburg College, Chemistry Department, Minneapolis, MN
- WP 546 **Stoichiometry of HIV-1 Gag Polyprotein-RNA Complexes as Determined by Native Mass Spectrometry;** Samantha H Hinckley¹; Erik D Olson¹; Karin Musier-Forsyth¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- WP 547 **Negative-Ion Mode RNA Top-down Mass Spectrometry for Revealing Interaction Sites within RNA-Protein Complexes;** Kevin M Ilek¹; Kristina Hakansson²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, MI
- WP 548 **Improved Mapping of Eukaryotic mRNA-binding Regions on Proteins using High Resolution Mass Spectrometry;** Meeli Mullari¹; David Lyon¹; Lars Juhl Jensen¹; Michael L Nielsen¹; ¹NNF CPR, Copenhagen
- WP 549 **RNA Modification Mapping Using Mass-to-Charge Dependent Collision Energies on a Synapt G2-S;** Peter A. Lobue¹; Balasubrahmanyam Addepalli¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- WP 550 **A Comparison of Positive and Negative Ion Collision-Induced Dissociation of 2'-O-Modified and Unmodified Phosphorothioate Oligonucleotides;** Jaeah Kim¹; Michael Bartlett²; ¹University of Georgia, Athens, GA; ²University of Georgia, Athens, GA
- WP 551 **LC/MS Oligonucleotide Mass Fingerprinting (OMF) Enables Rapid Characterization of Critical Quality Attributes in Therapeutic mRNA;** Serenus Hua¹; Srujan Kumar Gandham¹; Tao Jiang¹; Kerry Salandria¹; Chisom Udengwu¹; Ipsita Roymoulik¹; James D. Thompson¹; ¹Moderna Therapeutics, Cambridge, MA
- WP 552 **Two-Dimensional Liquid Chromatography-Mass Spectrometry for the Characterization of Oligonucleotide Impurities;** Stilianos G. Roussis¹; Claus Rentel¹; ¹Ionis Pharmaceuticals, Inc., Carlsbad, CA
- WP 553 **LC-MS Based Determination of Pseudouridine at Single Nucleotide Resolution in Mammalian Non-Coding RNAs using a Uridine Synthesis Deficient Cell line;** Yuko Yamaki¹; Yuko Nobe¹; Hiroshi Nakayama²; Hideaki Ishikawa³; Yoshio Yamauchi¹; Nobuhiro Takahashi³; Toshiaki Isobe¹; Masato Taoka¹; ¹Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; ²RIKEN Center for Sustainable Resource Science, Wako, Japan; ³Tokyo University of Agriculture and Technology, Fuchyu, Japan
- WP 554 **Mass Spectrometry and Next Generation Sequencing Analysis of tRNAs from the Pathogenic Fungi Cryptococcus Neoformans;** Mellie Paulines¹; Andrew Holmes²; Todd Lowe²; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH; ²University of California, Santa Cruz, Santa Cruz, CA
- WP 555 **Direct identification of miR-451 from plasma using LC-MS;** Babak Basiri¹; Michael Bartlett¹; ¹University of Georgia, Athens, GA
- WP 556 **Detection and Mapping of Post-Transcriptional tRNA Modifications in the Radioresistant Bacterium Deinococcus radiodurans;** Ruoxia Zhao¹; Patrick A Limbach²; ¹University of Cincinnati, Cincinnati, OH; ²University of Cincinnati, Cincinnati, OH
- WP 557 **Using LC/ESI-FTMS to Identify Cellular Damage Products within the RNA of a Radiotrophic Species;** Whitney Houser¹; Lauren Schultz¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- WP 558 **Rapid Genotyping of Oenantho Javanica and Cicuta virosa by Polymerase Chain Reaction Followed by Liquid Chromatography/Mass Spectrometry;** Hajime Miyaguchi¹; Tadashi Yamamuro¹; Daisuke Watanabe¹; Hikoto Ohta¹; ¹National Research Institute of Police Science, Kashiwa

- WP 559 **LC-MS/MS-based Quantitative Measurement of 8,5'-Cyclopurine-2'-Deoxynucleosides with Small Quantities of DNA;** Yuxiang Cui¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA
- WP 560 **Nonspecific Versus Specific Binding of Amino Acids and Dipeptides to RNA Probed by Electrospray Ionization and Collisionally Activated Dissociation;** Jovana Vusurovic¹; Kathrin Breuker²; ¹University of Innsbruck, Innsbruck, Austria; ²University of Innsbruck, Innsbruck, Austria
- WP 561 **Screening of DNA Adducts Induced by NNK and LPS Combined Exposures via a High Resolution LC-MS3 Adductomic Approach;** Andrea Carra¹; Peter W. Villalta¹; Romel P. Dator¹; Laura Maertens¹; Fekadu Kassie¹; Silvia Balbo¹; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN
- WP 562 **A Novel Approach for Detecting and Quantifying DNA Modification Using NanoLC-MS/MS;** Ranran Wu¹; Kevin Janssen¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- WP 563 **Affinity Selection Mass Spectrometry Enables Small Molecule Ribosome Binding Analysis;** Thomas O'Connell¹; Justin Stroh¹; Jason Ramsay²; Donna Petersen¹; Paula Loria¹; Bruce Maguire¹; ¹Pfizer, Groton, CT; ²Pfizer Inc, St Louis, MO

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- WP 564 **De Novo Sequencing of Peptides Derived from Scorpion Venom;** Meng Li¹; Yuko P. Y. Lam¹; Peng Chen²; Maria van Agthoven¹; Qiong Wu²; Mark P. Barrow¹; Hongzheng Fu²; Peter B. O'Connor¹; ¹University of Warwick, Coventry, UK; ²Peking University, Beijing, China
- WP 565 **Determination of the Prominent Fragment Ions Formed by Hot Electron Capture Dissociation (HECD) of Doubly-Charged Peptides and Tryptic Phosphopeptides;** Mark J. Raftery; ¹Bioanalytical Mass Spectrometry, Sydney, NSW
- WP 566 **Paleoproteomic Analysis of Early Pleistocene Fossil Remains;** Enrico Cappellini¹; Anna Katerina Fotakis¹; Rosa Rakownikow Jersie-Christensen²; David Lyon²; José Víctor Moreno Mayar¹; Maia Bukhsianidze³; Christian D. Kelstrup²; David Lordkipanidze³; Jesper Velgaard Olsen²; Eske Willerslev¹; ¹Natural History Museum of Denmark, University of Copenhagen, Copenhagen, Denmark; ²Novo Nordisk Foundation Center for Protein Research, Faculty of Health Sciences, University of Copenhagen, Copenhagen, Denmark; ³Georgian National Museum, Tbilisi, Georgia
- WP 567 **Expansion of the Brachylophosaurus canadensis Collagen I Sequence and Additional Evidence for the Preservation of Cretaceous Protein;** Elena R. Schroeter¹; Caroline J. DeHart²; Timothy P. Cleland³; Wenxia Zheng¹; Paul M. Thomas²; Neil L Kelleher²; Marshall Bern⁴; Mary H. Schweitzer¹; ¹North Carolina State University, Raleigh, NC; ²Northwestern University, Evanston, IL; ³University of Texas at Austin, Austin, TX; ⁴Protein Metrics Inc., San Carlos, CA
- WP 568 **Structural Characterization of Spider PeptidePha1β Using Mass Spectrometry Based Approaches;** Kelly L. Wormwood¹; Armand G. Ngounou Wetie¹; Marcus V. Gomez²; Costel C. Darie¹; ¹Clarkson University, Potsdam, NY; ²Institute of Education and Research Santa Casa Belo Horizonte-Laboratory of Toxins, Belo Horizonte, Brazil
- WP 569 **Rapid and Sensitive Phosphoproteomics on a Modified Q Exactive™ HF;** Dorte B. Bekker-Jensen¹; Christian D. Kelstrup¹; Tabiwang Arrey²; Alexander Hogrebe¹; Alexander Harder²; Jesper V. Olsen¹; ¹CPR, University of Copenhagen, Copenhagen, Denmark; ²Thermo Fisher Scientific, Bremen, Germany
- WP 570 **Low Dispersion Electrochemical Flow Cell for On-Line LC-EC-MS;** Martin Eysberg¹; Jean-Pierre Chervet²; Hendrik-Jan Brouwer²; Pablo Sanz de la Torre²; ¹Antec Scientific



- (USA), Boston, MA; ²Antec Scientific, Zoeterwoude, Netherlands
- WP 571 **LC-MS Method to Evaluate Incidence Rate of Protein Sequence Variants in Biopharmaceuticals;** Heather Oakes¹; Sylwia Jozwiak¹; Marc Feary²; Frances Kenny¹; Steve Flatman¹; James Graham¹; ¹Lonza Biologics, Slough, Berkshire; ²Lonza Biologics, Cambridge, UK
- WP 572 **Identification and Localization of Modified Residues in Disulfide-Linked Peptides via CID of Anionic Species;** Alice L. Pilo¹; Weijuan Tang¹; ¹Merck & Co., Inc, Rahway, NJ
- WP 573 **Proteogenomic Analyses of Neoantigen Diversity in Cisplatin-Resistant Ovarian Cancer Cells;** Nicholas W. Bateman^{1,2}; Guisong Wang¹; Brian L. Hood¹; Chad A. Hamilton^{1,3}; George L. Maxwell^{1,4}; Thomas P. Conrads^{1,4}; ¹WHIRC, Annandale, VA; ²The John P. Murtha Cancer Center, Walter Reed National Military Medical Center, Bethesda, MD; ³Gynecologic Oncology Service, Walter Reed National Military Medical Center, Bethesda, MD; ⁴Inova Schar Cancer Institute, Falls Church, VA
- WP 574 **A Systematic and Quantitative Study on Kinetics of Immobilized Trypsin Based Protein Digestion;** Xiaojing Shen¹; Daoyang Chen¹; Liangliang Sun¹; ¹Michigan State University, Lansing, MI
- WP 575 **SWATH-MS-Data Independent Acquisition Strategies for Ultimate Confidence in Peptide Mapping and Post Translational Modifications quantitation for Biotherapeutics Characterization;** Sibylle Heidelberger¹; Annu Uppal²; ¹SCIEX, Concord, ON, Canada; ²Sciex, India, Gurgaon, India
- PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS II**
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- WP 576 **Targeted Proteomics Analysis of Epithelial to Mesenchymal Transition Biomarkers in Cancer;** Vitor Faca¹; Camila Palma¹; Mariana Grassi¹; Guilherme Lanfredi¹; Germano Ferreira¹; Carolina Thome¹; Aline Poersch¹; ¹Ribeirao Preto Medical School - University of Sao Paulo, Ribeirao Preto, Brazil
- WP 577 **Analysis of Amyloid-Beta Isoform Composition in Human Blood Plasma and Platelets;** Anna Bugrova¹; Maria I. Indeykina^{1,2,3}; Natalia V. Zakharova¹; Alexey S. Kononikhin²; Stanislav I. Pekov^{2,3}; Igor Popov^{1,2}; Sergey A. Kozin⁴; Eugene (Evgeny) Nikolaev^{2,5,6}; ¹Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; ²Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ³Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; ⁴Engelhardt Institute of Molecular Biology, Moscow, Russia; ⁵Skolkovo institute of science and technology, Skolkovo, Russia; ⁶Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia
- WP 578 **Quantitation of Low-Level Peptide Impurities in Certified Reference Materials and Incorporation of Ion Mobility Mass Spectrometry for Conformational Isomer Characterization;** Bradley Stocks¹; Marie-Pier Thibeault¹; Juris Meijja¹; Jeremy Melanson¹; ¹National Research Council Canada, Ottawa, ON, Canada
- WP 579 **"Shotgun Microdialysis" with LC-MS3 Quantitation for the Screening of BBB Penetration Properties of Peptide-Based Drugs;** Catherine Kramer¹; Mitchell J. Bartlett¹; Evan M. Jones¹; Chris Stagg¹; Robin Polt¹; Torsten Falk¹; Michael L. Heien¹; ¹University of Arizona, Tucson, AZ
- WP 580 **Development of a Sensitive Method (pM levels) for a Lipidated Peptide in Rat Plasma Using Hybrid Immuno-affinity Purification with LC-MS/MS;** Cynthia M. Chavez-Eng¹; Dina Goykhman¹; Yifan Song¹; ¹Merck & Co., Inc, Kenilworth, NJ
- WP 581 **Improved Solid-Phase Extraction Protocol and Sensitive Quantification of Six Microcystins in Water using an HPLC-orbitrap Mass Spectrometry System;** Dilrukshika S. W. Palagama¹; Raymond E West III²; Dragan Isailovic²; ¹The University of Toledo, Toledo, OH; ²University of Toledo, Toledo, OH
- WP 582 **The Application of Targeted Proteomics for Investigating Organic Cation Transporter Protein Mediated Drug-Drug Interaction Between Rifampicin and Metformin;** Katya Govender^{1,2}; John Howard Adamson²; Peter Owira¹; ¹University of Kwazulu-Natal, Durban, South Africa; ²Africa Health Research Institute (AHRI), Durban, South Africa
- WP 583 **Development of a PRM Method to Quantify HLA Class I Peptides in Leukemia Cells;** Laura Herring^{1,2}; Sally Hunsucker³; Courtney Elliott³; Lee Graves^{1,2,3}; Gianpietro Dotti^{3,4}; Paul Armistead^{3,5}; ¹Department of Pharmacology, UNC-Chapel Hill, Chapel Hill, NC; ²UNC Proteomics Core Facility, UNC-Chapel Hill, Chapel Hill, NC; ³Lineberger Comprehensive Cancer Center, Chapel Hill, NC; ⁴Department of Microbiology and Immunology, UNC-Chapel Hill, Chapel Hill, NC; ⁵Department of Medicine, UNC-Chapel Hill, Chapel Hill, NC
- WP 584 **Improved Quantification of the Therapeutic Peptide Liraglutide in Human Plasma;** Mark David Platt¹; Damon I. Papac¹; ¹ICON Bioanalytical Laboratories, Clinton, NY
- WP 585 **Comparison of Mass Spectrometric Immunoassay and Magnetic Beads Assay for Quantitation of Peptide in Rat and Dog Plasma with LC/MS/MS;** Ming Wang¹; Yang Xu¹; Tonya Jackson¹; Steven Bucher¹; Danny Choo¹; Helengrace Schuck¹; Xiang Yu¹; James Schiller¹; ¹Pharmacokinetics, Pharmacodynamics and Drug Metabolism, Merck Research Laboratories, Merck & Co., Inc., West Point, PA
- WP 586 **HPLC-QqOrbitrap Analyses Reveal a Significant Reduction of Tachykinin and Opioid Neuropeptides Level in PC1 and PC2 Mutant Mouse Spinal Cords;** Mouna Saidi¹; Soufiane Kamali¹; Francis Beaudry¹; ¹Université de Montréal, St-Hyacinthe, QC, Canada
- WP 587 **Extraction of MC-LR from Serum and its Quantification by LC-ESI-Orbitrap-MS;** Rachel K Marvin¹; Dilrukshika S. W. Palagama¹; David Balu-Rodriguez¹; Bruce S. Levison¹; Judy Westrick²; David Kennedy¹; Kenneth Hensley³; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH; ²Wayne State University, Detroit, MI; ³Arkansas College of Osteopathic Medicine, Fort Smith, AR
- WP 588 **Understanding Cellular Drug Response by Measuring Apoptosis Pathway Members using the TOMAHQ assay;** Robert A. Everley¹; Kartik Subramanian¹; John A. Bachman¹; Brian K. Erickson¹; Alison R. Erickson¹; Matthew J. Berberich¹; Christopher M. Rose²; Jeffery Knott³; Caitlin E. Mills¹; Yvonne Hua¹; Mirra Chung¹; Steven P. Gygi¹; Peter K. Sorger¹; ¹Harvard Medical School, Boston, MA; ²Genentech, Inc., South San Francisco, CA; ³Cell Signaling Technologies, Danvers, MA
- WP 589 **A SRM/MS/MS Based Targeted Proteomics Strategy for Quantification of Potential Biomarkers of TKI Sensitivity in EGFR Mutated Lung Adenocarcinoma;** Shivangi Awasthi^{1,2}; Tapan Maity¹; Xu Zhang¹; Benjamin L. Oyler³; David R. Goodlett²; Udayan Guha¹; ¹Thoracic & Gastrointestinal Oncology Branch, CCR, NCI, Bethesda, MD; ²School of Pharmacy, University of Maryland, Baltimore, MD; ³Institute of Marine and Environmental Technology, University of Maryland Center for Environmental Science, Baltimore, MD
- WP 590 **Application of MALDI-TOF-MS for Improvement of Quantitative Determination of α - and β -Asp7 Isoforms of amyloid- β Peptide for Alzheimer's Disease Diagnostics;** Stanislav Pekov^{1,2}; Maria Indeykina^{2,3}; Anna Bugrova³; Alexey Kononikhin^{1,2,3,4}; Igor Popov^{1,2}; Eugene (Evgeny) Nikolaev^{1,2,5}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; ³Emanuel Institute of Biochemical Physics of



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- WP 591 **Human Tissue Distribution of Carbonyl Reductase 1 Using Proteomic Approach with LC-MS/MS;** Wenyi Hua¹; Hui Zhang¹; Sangwoo Ryu¹; Xin Yang¹; Li Di¹; ¹Pfizer Inc., Groton, CT
- WP 592 **Targeted Proteogenomics of Outer Membrane Vesicles Mediating Antibiotic Resistance Transfer among the Acinetobacter;** William Judson Hervey, IV¹; Scott A. Walper¹; Kendrick B. Turner¹; ¹Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC
- WP 593 **Middle-Down Analysis of Muropeptides Alteration in Stenotrophomonas maltophilia Cell Wall;** Yun Lin¹; Yi-Wei Huang²; Chin Lin³; Yu Wang^{2,4}; Yi-Tsung Lin^{5,6}; Tsuey-Ching Yang²; Cheng-Chih Richard Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan; ³School of Public Health, National Defense Medical Center, Taipei, Taiwan; ⁴Department of Laboratory Medicine, Chang Gung Memorial Hospital Linkou Branch, Taoyuan, Taiwan; ⁵Division of Infectious Diseases, Department of Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; ⁶School of Medicine, National Yang-Ming University, Taipei, Taiwan
- WP 594 **Rapid Screening of Peptide Impurities in Calcitonin-Salmon Nasal Spray Using Data-Dependent LC-MS-MS;** Jingyue Yang¹; Priyanka Chitranshi¹; Ilan Geerloff-Vidavsky¹; Kui Zeng¹; David A. Keire¹; Michael Trehly¹; Wenlei Jiang²; Deyi Zhang²; Xiaohui Jiang²; Daniela Verthelyi³; ¹Division of Pharmaceutical Analysis, Office of Testing and Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO; ²Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD; ³Office of Biotechnology Products, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD

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- WP 595 **Selective Isolation of Tyrosine-Phosphorylated Protein by Magnetic Nanoparticles Composites;** Meng-han Liu¹; He-Hsuan Hsiao¹; ¹Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan
- WP 596 **Automated High-Throughput Phosphopeptides Enrichment using TiO₂ Dispersive Pipette Extraction;** Sunil Hwang¹; Todd Mulis¹; Jingyun Lee²; Michael Mouridian³; Cristina Furdut²; Andrew Lee¹; ¹Integrated Micro-Chromatography Systems, LLC, Irmo, SC; ²Proteomics and Metabolomics Shared Resource, Wake Forest School of Medicine, Winston-Salem, NC; ³Hamilton Robotics, Reno, NV
- WP 597 **High-throughput Workflow For Deep Phosphoproteome Analysis;** Yun-Chien Chang^{1,2}; Reta Birhanu Kitata^{1,3}; Pei-Yi Lin¹; Yu-Ju Chen^{1,2}; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ²Department of Chemistry, National Taiwan University, Taipei, Taiwan; ³Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan
- WP 598 **Robust, Sensitive, and Automated Phosphopeptide Enrichment Optimized for Low Sample Amounts Applied to Primary Hippocampal Neurons;** Harm Post¹; Renske Penning²; Martin A. Fitzpatrick²; Luc B. Garrigues²; Wei Wu²; Harold D. MacGillavry²; Casper C. Hoogenraad²; Albert J. R. Heck²; A.F. Maarten Altaar²; ¹, Utrecht, Utrecht; ²Utrecht University, Utrecht, Netherlands
- WP 599 **A Combined Enrichment/Enzymatic Approach to Study Phosphoproteomics "Dark Matter.";** Evgeny Kanshin¹; Mirela Pascariu¹; Mike Tyers¹; Damien D'Amours¹; Pierre Thibault¹; ¹IRIC-Université de Montréal, Montréal, QC, Canada
- WP 600 **Enrichment of Phosphopeptides Using Poly-L-Lysine-Encapsulated Sol-Gel Material;** Ülkü Güler Tokat¹; Mehmet Atakay²; Hacı Mehmet Kayili^{3,4}; Bekir Salih²; ¹Hacettepe University, Department of Chemistry, Ankara, Cankaya; ²Hacettepe University, Department of Chemistry, Ankara, Cankaya; ³Department of Chemistry, Çankırı Karatekin University, Çankırı, Turkey; ⁴Department of Nutrition and Dietetics, Karabük University, Karabük, Turkey
- WP 601 **SMOAC (Sequential Enrichment from MOAC, "Smoke"), A Phosphoproteomics Enrichment Strategy for the Separation of Multiply Phosphorylated from Monophosphorylate;** Jae Choi¹; Sergei Snovidia¹; Ryan Bomgarden¹; John C. Rogers¹; ¹Thermo Fisher Scientific, Rockford, IL
- WP 602 **Quantitative Phosphoproteomics of the Protein Phosphatase 2 Complex Using the Chip iFunnel QTOF Platform;** Paulos Chumala¹; Brooke Thompson¹; Vadiraja Bhat²; Chelsea E. Cunningham³; Frederick S. Vizeacoumar³; Franco J. Vizeacoumar⁴; George S. Katselis¹; ¹CCHSA/Department of Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada; ²Agilent Technologies, Inc., Wilmington, DE; ³Department of Pathology, Cancer Cluster, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada; ⁴Department of Pathology, Cancer Cluster, College of Medicine, University of Saskatchewan and Cancer Research, Saskatchewan Cancer Agency, Saskatoon, SK, Canada
- WP 603 **A Simple Assay to Determine the Amount of Titanium Dioxide Required for Maximum Enrichment of Phosphopeptides;** Alissa Schunter¹; Jeffrey R. Anderson²; Young Ah Goo¹; Paul Thomas²; Neil L Kelleher²; ¹Northwestern University, Chicago, IL; ²Northwestern University, Evanston, IL

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- WP 604 **Characterization of the Adsorption-Desorption Properties of Polystyrene Microspheres Using Paper Spray Mass Spectrometry;** Yajun Zheng¹; Teng Wang¹; Xiaoting Wang¹; Zhiping Zhang¹; ¹Xi'an Shiyu University, Xi'an, China
- WP 605 **Analysis of nylon-6 by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS) and Pyrolysis-GC/MS;** Chikako Takei¹; Kenichi Yoshizawa¹; Hajime Ohtani²; ¹BioChromato, Inc., Fujisawa, Japan; ²Nagoya Institute of Technology, Nagoya, Japan
- WP 606 **Energetic Fluorinated Polymers Characterization: Novel Combination of ASAP-Orbitrap MS and Kendrick Mass Defect Analyse;** Gabriel Gaiffe¹; Richard B. Cole¹; Sabrina Lacpatia²; Maxime C. Bridoux³; ¹Sorbonne Universités UPMC, Paris, France; ²Laboratoire Central de la Préfecture de Police, Paris, France; ³CEA, DAM, DIF, Arpajon, France
- WP 607 **Micelles Protect Hydrophobic Metallo-supramolecules from Water to Electrospray Ionization Mass Spectrometry in Their Native States;** Kai-Hung Huang¹; Tsung-Han Tu¹; Shi-Cheng Wang¹; Sheng-Tao Chang¹; Yi-Tsu Chan¹; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan
- WP 608 **Surface Analysis using Solvent-Free Silver-Nanoparticle Surface-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging;** Takaya Satoh¹; Naoki Kikuchi¹; Hironobu Niimi¹; Makiko Fujii²; Toshio Seki³; Jiro Matsuo³; Michael H. Frey⁴; ¹JEOL Ltd., Akishima, Japan; ²Yokohama National University, Yokohama, Japan; ³Kyoto University, Uji, Japan; ⁴JEOL USA Inc., Peabody, MA



- WP 609 **Structural and Biological Characterization of Degradation Products Generated during Radical Depolymerization of Hyaluronan**; Martina Hermannova¹; Dagmar Cozikova¹; Radovan Buffa¹; Kristina Nesporova¹; Vladimir Velebny¹; ¹Contipro a.s., Dolni Dobrouc, Czech Republic
- WP 610 **The first Observation of High Mass Distribution of Polyrotaxane using MALDI-TOFMS and a High Mass Detector**; Shuuichi Nakaya¹; Kazuaki Kato²; Yuzo Yamazaki¹; Kohzo Ito²; ¹Shimadzu Corporation, Kyoto, Japan; ²Department of Advanced Material Science, Graduate School of Frontier Science, The University of Tokyo, Japan
- WP 611 **Why are Electron Ionization Mass Spectra of Phenyl Methyl Cyclosiloxane Polymers So Difficult to Interpret?**; Tanya Habitz¹; Ron Tecklenburg¹; Amanda Palumbo¹; ¹Dow Corning Corporation, Auburn, MI
- WP 612 **MS/MS Assisted Design to Improve Readability of Messages Chemically Encoded in Sequence-Defined Copolymers**; Laurence Charles¹; Gianni Cavallo²; Laurence Oswald²; Rosa Szveda²; Jean-Francois Lutz²; ¹Aix-Marseille University, Marseille Cedex 20, France; ²Institut Charles Sadron, CNRS, Strasbourg, France
- WP 613 **Determination of the Detailed Electron Ionization Fragmentation Pathways for Trifluoropropyl Containing Siloxane Polymers. Evidence for Si-F Bond Formation**; Ron Tecklenburg¹; Tanya Habitz¹; Amanda Palumbo¹; ¹Dow Corning Corporation, Auburn, MI
- WP 614 **Analysis of Sequence-Defined Polyester Copolymers by MALDI Tandem Mass Spectrometry**; Jialin Mao¹; Chrys Wesdemiotis¹; Wei Zhang¹; Stephen Z.D. Cheng¹; ¹The University of Akron, Akron, OH
- WP 615 **Analysis of Positional Poly(Pyridylalkyl Methacrylate) Isomers and Homologs by Fragmentation and Ion Mobility Mass Spectrometry**; Michelle Kushnir¹; Chrys Wesdemiotis¹; Marios Elladiou²; Costas S. Patrickios²; ¹University of Akron, Akron, OH; ²University of Cyprus, Nicosia, Cyprus
- WP 616 **Effective Method for Lignin Molecular Weight Determination: High Resolution Mass Spectrometry or Size Exclusion Chromatography?**; Anastasia A. Andrianova¹; Thomas DiProspero¹; Clayton Geib¹; Irina P. Smoliakova¹; Evguenii I. Kozliak¹; Alena Kubátová¹; ¹Chemistry Department, University of North Dakota, Grand Forks, ND
- WP 617 **Identification of Novel Print-Related Contaminants in Polymeric Food Packaging**; Miguel A. Lago¹; Luke K Ackerman²; ¹University of Santiago de Compostela, Santiago de Compostela, Spain; ²FDA/CFSAN, College Park, MD
- WP 618 **Non-Targeted Screening of Extractables and Leachables in E-cigarettes using a Single Platform UPLC-APGC-QTOF-MS**; Naren Meruva¹; Baiba Cabovska¹; Steven Lai²; Dimple Shah¹; Kari Organtini¹; Gareth Cleland¹; Kenneth Rosnack¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Beverly, MA
- WP 619 **On-Surface Analysis of Oligomeric Intermediates during Bottom-Up Fabrication of Graphene Nanoribbons by Mass Spectrometry**; Hans Joachim Raeder¹; Wen Zhang¹; Zongping Chen¹; Klaus Müllen¹; ¹MPI for Polymer Research, Mainz, Germany
- WP 620 **Quantitation and Identification of Polysorbates in Protein Matrix**; Pengxiang Yang¹; Kerry M Hassell²; Christopher Elicone³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Somerset, NJ; ³Thermo Fisher Scientific, Franklin, MA
- WP 621 **Analytical Uncertainty and Response Factors for Extractable and Leachable Analysis using LCMS**; Dujuan Lu¹; Kate Comstock²; ¹SGS Life Science Service, Fairfield, NJ; ²Thermo Fisher Scientific, San Jose, CA
- WP 622 **Sample Productive Method for Low Boiling Point Compound and Rapid Analysis of Phthalic Acid Esters in DIP/MS using Fragmentless Ionization**; Takahisa Tsugoshi¹; Yuji Mishima²; ¹AIST, Tsukuba; ²Kobe Material Testing Laboratory Co., Ltd., Taito-ku, Japan
- WP 623 **Single-Use Biobag Extractable Analysis Using LC-HRMS**; Colin Barry¹; Kate Comstock²; Darlene Murphy³; ¹Alliance Pharma, Malvern, PA 19355; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA
- WP 624 **Fragmentation Rules of Poly(lactide)s in Collision-Induced Dissociation**; Christophe Chendo¹; Marion Rollet¹; Trang Phan¹; Didier Gimes¹; Laurence Charles¹; ¹Aix-Marseille University, Marseille, France
- WP 625 **Profiling Extractables from 3D Printed Structures Prepared Using Additive Manufacturing Techniques**; Maruti Hedge^{1,2}; Allison M. Pekkanen^{1,2}; Timothy E Long^{1,2}; Andrew Baker³; ¹Virginia Tech Department of Chemistry, Blacksburg, VA; ²Macromolecular Innovation Institute, Blacksburg, VA; ³Waters, Inc., Pleasanton, CA

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- WP 626 **A Streamlined Workflow for the Rapid Quantification of Biotherapeutic Antibodies**; Michael Rosenblatt¹; Nidhi Nath²; Sergei Saveliev²; Marjeta Urh²; ¹Promega Corp, Madison, WI; ²Promega Corporation, Madison, WI
- WP 627 **Quantification of Total Antibody from an ADC in Monkey Plasma using Hybrid LBA-LCMS Techniques: Triple Quadrupole vs HRMS (Orbitrap) Comparison**; Eric Ma¹; Mocun Yuan¹; William Mylott¹; Rand Jenkins¹; ¹PPD Laboratories, Richmond, VA
- WP 628 **Quantification of a Monoclonal Antibody in Nasal Lavage by LC-MS/MS with Abundant Protein Normalization**; Ryan Lutz¹; Daniel S. Spellman¹; Kevin P. Bateman¹; ¹Merck & Co., Inc., West Point, PA
- WP 629 **High Sensitivity Quantification of Intact therapeutic Proteins derived from Plasma Using a High-Resolution QToF Mass Spectrometer**; Henry Shion¹; Yun Alelyunas²; Gregory Roman²; Nigel Ewing²; Mark Wrona²; Ying-Qing Yu²; Weibin Chen²; ¹Waters Corp, Milford, MA; ²Waters Corp, Milford, MA
- WP 630 **Statistical Characterization of Therapeutic Protein Modifications**; Tsung-Heng Tsai¹; Zhiqi Hao²; Qiuting Hong^{2,3}; Benjamin Moore²; Cinzia Stella²; Jeffrey H. Zhang²; Yan Chen²; Michael Kim²; Theo Koulis²; Gregory A. Ryslik²; Erik Verschueren²; Fred Jacobson²; William E. Haskins²; Olga Vitek¹; ¹Northeastern University, Boston, MA; ²Genentech, Inc, South San Francisco, CA; ³Eurofins Lancaster Laboratories, Inc., Lancaster, PA
- WP 631 **Software Platform for Automated Peptide Mapping: Application to Rapid Critical Quality Attribute Identification and Quantitation for Early Developability Assessment**; David R Bush¹; Joe Shambaugh¹; Stefano Gotta²; Maurizio Bronzetti¹; Cassandra Wigmore¹; Arnd Brandenburg²; ¹Genedata Inc, Lexington, MA; ²Genedata AG, Basel, Switzerland
- WP 632 **Evaluation of Coated Microplates for Recovery of Therapeutic Proteins and Peptides**; Bao-Jen Shyong¹; Ryan Lutz¹; Daniel S. Spellman¹; KEVIN P. Bateman¹; ¹Merck Research Labs, Merck & Co., West Point, PA
- WP 633 **Development of an Affinity Capture-LC-MS/MS Assay for the Quantitation of Adalimumab in Human Plasma using BioBA sample preparation kit**; Jean-François Dupuis¹; Kevork Mekhssian¹; Ian Moore²; Anahita Keyhani¹; ¹Altasciences, Laval, QC, Canada; ²SCIEX, Concord, ON, Canada, Canada
- WP 634 **Robust sub-ng/mL Sensitivity for Protein Biotherapeutics Quantification without Immunoaffinity**



- WP 635 **Enrichment, using a Novel and Universally-Applicable Dual-Mechanism Enrichment Strategy;** Bo An¹; Ming Zhang¹; Yang Qu¹; Jun Qu¹; ¹*SUNY at Buffalo, Buffalo, NY*
- WP 636 **Identification and Quantification of Post-Translational Modifications in Therapeutic Monoclonal Antibodies by Peptide Mapping using the NISTmAb High-Resolution Spectral Library;** Qian Dong¹; Xinjian Yan¹; Yuxue Liang¹; Yuri Mirokhin¹; Sanford P. Markey¹; Tallat Bukhari¹; Stephen E Stein¹; ¹*NIST, Gaithersburg, MD*
- WP 637 **MRM Assays to Assess Presence of a Host Cell Protein Contaminant Impacting Monoclonal Antibody Drug Product Stability;** Lie Min¹; Josephine Chiu¹; Kelvin H. Lee¹; ¹*Department of Chemical and Biomolecular Engineering and Delaware Biotechnology Institute, University of Delaware, Newark, DE*
- WP 638 **Sensitive and Robust Quantitation of Intact Monoclonal Antibody using A Newly Developed Q-TOF Instrument;** Alex ZHU¹; David Wong²; Aaron Boice²; ¹*Agilent Technologies, Wilmington, DE*; ²*Agilent Technologies, Santa Clara, CA*
- WP 639 **Enhanced Detection Sensitivity of Protein Therapeutics in Human Serum using Multi-Nozzle Emitters Coupled with capillary UPLC – Quantiva;** Yao-Yun Fan¹; Jianxia Shi¹; Pan Mao²; Geuncheol Gil²; Daojing Wang²; Dan Rock¹; Ji Ma¹; ¹*Amgen, South San Francisco, CA*; ²*Newomics Inc., Emeryville, CA*
- WP 640 **Regulated LC/MS/MS Bioanalysis of Therapeutic Antibodies Based on Nano-Surface and Molecular-Orientation Limited (nSMOL) Proteolysis Method using a New Reagent Kit;** Toshiya Matsubara¹; Noriko Iwamoto²; Deepti Bhandarkar³; Masateru Oguri¹; Rashi Kochhar³; Takashi Shimada²; Ichiro Hirano¹; ¹*Shimadzu Corporation, Kyoto, Japan*; ²*Shimadzu Corporation, Chuo-ku, Japan*; ³*Shimadzu Analytical India Pvt. Ltd., Mumbai, Maharashtra*
- WP 641 **Direct Quantitation of Intact mAb PTM Using Ultra High Resolution LC-MS SIM;** Xiaomei (Annie) He¹; Wanlu Qu¹; Chen Li¹; Janet Lau¹; Dongdong Wang¹; Billy Wu¹; ¹*BioAnalytix, Cambridge, MA*
- WP 642 **Simultaneous Quantitation and Catabolite Identification of Intact Proteins in Biological Samples using LC-HRMS;** Lijuan Kang¹; Naidong Weng¹; Wenying Jian¹; ¹*Janssen Research&Development, Spring House, PA*
- WP 643 **Targeted, Site-specific Quantitation of N- and O-Glycopeptides of Biologics using 18O-Labeling and Product Ion Based Mass Spectrometry;** Jandhyam Srikanth¹; Rathinasamy Agalyadevi¹; Ponnusamy Babu¹; Annu Uppal²; ¹*National Centre for Biological Sciences, Glycomics and Glycoproteomics & Biologics Characterization Facility, Bangalore, India*; ²*SCIEX, Gurgaon, India*
- WP 644 **A Simple Workflow for Monoclonal Antibody N-Glycan Analysis by LC-FLD-SQ;** Oscar Potter¹; Gregory O. Staples¹; Maggie Ostrowski¹; Hongfeng Yin¹; Kevin Killeen¹; ¹*Agilent Technologies, Santa Clara, CA*
- WP 645 **Improved Multiplexed Comparative Analysis of Intact Glycopeptides from Imiglucerase and Velaglucerase Alfa using ETD and SPS MS3;** Hongbin Zhu¹; Chen Qiu¹; David A. Keire¹; Hongping Ye¹; ¹*Division of Pharmaceutical Analysis, Office of Testing and Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO*
- WP 646 **Monitoring Changes in Glycosylation during the Production of Biotherapeutics in Plants - Butyrylcholinesterase (BChE) Expressed in Tobacco and Rice Systems;** Muchena J. Kallemba¹; Jasmine M. Corbin¹; Salem Al-Kanaimsh¹; Qiongyu Li¹; Kalimuthu Karuppanan¹; Li Yanhong¹; Raymond L. Rodriguez¹; Xi Chen¹; Somen Nandi¹; Karen McDonald¹; Carlito B. Lebrilla¹; ¹*University of California, Davis, Davis, CA*
- WP 647 **Data Independent Acquisition LC-MS Strategy;** Søren Heissel¹; Jakob Bunkenborg²; Thomas Kofoed²; Marie Grimstrup²; Anne Fich Holmberg³; Max Per Kristiansen³; Ingrid Kromann³; Ejvind Mørtz²; Peter Højrup¹; ¹*University of Southern Denmark, Odense M*; ²*Alphalyse A/S, Odense, Denmark*; ³*Statens Serum Institut, Copenhagen, Denmark*
- WP 648 **LC-MS Based HCP Monitoring During Biologic Downstream Process Development;** Chen Li¹; Wanlu Qu¹; Serah Liu¹; Shiaw-Lin Wu¹; Fengqiang Wang²; Yan-Hui Liu²; Doug Richardson²; Daisy Richardson²; ¹*BioAnalytix, Inc., Cambridge, MA*; ²*Merck & Co., Inc, Kenilworth, NJ*
- WP 649 **An Improved, Selective Trapping Micro-LC/MS for Ultra-Sensitive, Robust and High-Throughput Quantification of Biotherapeutics and Biomarkers in Plasma and Tissues;** Bo An¹; Ming Zhang¹; Yang Qu¹; Jun Qu¹; ¹*SUNY at Buffalo, Buffalo, NY*
- WP 650 **Development of a Multi-Peptide Immunocapture – LC-MS/MS Assay for the Quantitation of a Pegylated Therapeutic in Rat and Dog Plasma;** Kevoork Mekhssian¹; Jean-François Dupuis¹; Olivier Didur²; William Ruddock²; Anahita Keyhani¹; ¹*Algorithm Pharma, Laval, QC, Canada*; ²*ITR Laboratories, Montreal, QC, Canada*
- WP 651 **Quantification of Calmodulin Like Protein using Immobilized Metallic Affinity Chromatography on the AB SCIEX Triple TOF 5600+;** Mathew Hautman¹; Yong Xi Li¹; Yan Ke¹; Nelson Santiago¹; ¹*Medpace Inc., Cincinnati, OH*
- WP 652 **Quantification of Grass Pollen and Mite Allergens by Mass Spectrometry: ICH Validated Methods Applied to Immunotherapy Drug Products;** Emmanuel Nony¹; Maxime Le Mignon¹; Armelle Martelet¹; Matthieu Rouet¹; Sandrine Riandé¹; Christel Dayang¹; Philippe Moingeon¹; ¹*Stallergenes Greer, Antony, France*
- WP 653 **An Epitope Imprinting Method for Specific Purification of Targeted Proteins;** Chao-Yu Hsiao¹; He-Hsuan Hsiao¹; ¹*Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan*
- WP 654 **Versatile Enzyme Activity Assay of a PEGylated Cyst(e) inase in Mammalian Sera Using LC-MS/MS;** Laurence M. Brill¹; Susan Alters²; Everett Stone³; Michael H. Buonarati¹; Dale Schoener¹; ¹*Intertek Pharmaceutical Services, San Diego, CA*; ²*Aeglea Biotherapeutics, Austin, TX*; ³*University of Texas, Austin, TX*
- WP 655 **Determination of Ligand Number and Distribution in Intact Protein Conjugates with High Mass MALDI-TOF-MS;** Christopher C. Lai¹; James A. Kelley¹; Yongdong Wang²; Don Kuehl²; ¹*National Cancer Institute-Frederick, Frederick, MD*; ²*Cerno Bioscience, Norwalk, CT*
- WP 656 **Accurate Quantification of Trisulfide Bond Linkage Present in a Model Protein using Low pH Digestion Condition;** Tasneem Bahrainwala¹; Mandy Xie¹; Nicholas Bond²; Brian Russell¹; Timothy Pabst¹; Xiangyang Wang¹; ¹*Medimmune Ilc, Gaithersburg, MD*; ²*Medimmune Ilc, Cambridge, UK*
- WP 657 **Overcoming Challenges Encountered During LC-MS and LC-MS/MS Stability Analysis of Co-Formulated Proteins and Peptides;** JASON X. TANG¹; Amber Peariso¹; ¹*Eli Lilly & Company, Branchburg, NJ*
- WP 658 **Improved Sensitivity for LC-MS Quantitation of Biologics in Plasma using Trap-and-Elute MicroLC-MS;** Remco van Soest¹; Khaterah Motamedchaboki¹; Sibylle Heidelberger²; Ian Moore²; ¹*SCIEX, Redwood City, CA*; ²*Sciex, Concord, ON, Canada*
- WP 659 **An Automated Procedure for the Optimization of High Resolution Accurate Mass Processing Methods for Quantitative Bioanalysis;** Keeley Murphy¹; Iman Mohtashemi²; Mark Sanders²; Jonathan L. Josephs²; ¹*Thermo Fisher Scientific, Cambridge, MA*; ²*ThermoFisher, San Jose, CA*



- WP 659 **Development of Bioanalytical Method for Determination of Intact Human Insulin from Plasma using LC/MS/MS;** Deepthi Bhandarkar¹; Ashutosh Shelar¹; Vikas Trivedi²; Tulsidhas Mishra²; Abhishhek Gandhi²; Swati Guttikar²; Toshiya Matsubara³; ¹*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*; ²*Veeda Clinical Research Pvt. Ltd., Ahmedabad, India*; ³*Shimadzu Corporation, Kyoto, Japan*
- WP 660 **Comparison of Innovator and Biosimilar Filgrastim Through LC-MS/MS, IM-MS and Gas-phase Unfolding Data Analysis;** Jukyung Kang¹; Yuwei Tian¹; K. Ilker Sen²; Eric Carlson²; Brandon T Ruotolo¹; Anna Schwendeman¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Protein Metrics Inc., San Carlos, CA*
- WP 661 **Molecular Properties Based LC-MS/MS Method Development for Quantitative Analysis of Therapeutic Proteins;** Jing Man Wong¹; Xiaomeng Shen¹; Dan Rock¹; Jianxia Shi¹; ¹*Amgen, South San Francisco, CA*
- WP 662 **A Promising Alternative to SRM-Very-High-Resolution Selected-Ion- Monitoring (vHR-SIM@500k) Enables Ultra-Sensitive and Selective Biotherapeutics Quantification;** Bo An¹; Ming Zhang¹; Yuan-ju Chen¹; Jun Qu¹; ¹*SUNY at Buffalo, Buffalo, NY*

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- WP 663 **Identification of Tissue-Specific Antigens of Taenia Solium Cysts through Quantitative Multiplexed Proteomics;** Jose Navarrete-Perea¹; Marta Isasa²; Joao Paulo²; Ricardo Corral-Corral³; Jeanette Flores-Bautista¹; Gladis Fragoso¹; Raul J. Bobes¹; Edda Sciutto¹; Xavier Soberon⁴; Steven Gygi²; Juan P. Lacleite¹; ¹*Institute for Biomedical Research, UNAM, Mexico City, México, D.F.*; ²*Harvard Medical School, Boston, MA*; ³*Institute for Cellular Physiology, Mexico City, Mexico*; ⁴*Institute for Biotechnology, UNAM, Cuernavaca, Mexico*
- WP 664 **Proteogenomics Reveals Strain-Specific Peptides from Clinical Isolates of Mycobacterium Tuberculosis in South African Populations;** Tiaan D. J. Heunis¹; Anzaan Dippenaar¹; Paul D. van Helden¹; Nicolaas C. Gey van Pittius¹; Arnab Pain²; Robin M. Warren¹; Samantha L. Sampson¹; David Lee Tabb¹; ¹*Stellenbosch University Faculty of Medicine and Health Sciences, Cape Town, South Africa*; ²*King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*
- WP 665 **A Targeted Mass Spectrometry Assay for Detection of HIV Gag Protein Following Induction of Latent Viral reservoirs;** Daniela M Schlatter¹; Aiman A. Haqqani²; Xiaolin Li²; Mark R. Chance²; John C. Tilton²; ¹*Case Western Reserve University, Cleveland , OH*; ²*Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH*
- WP 666 **Identifying Toll-Like Receptor 2 Protein Interaction Partners using Quantitative Proteomics;** Abu Hena M Kamal¹; Saiful M. Chowdhury¹; ¹*University of Texas at Arlington, Arlington, TX*
- WP 667 **Rapid and Accurate Differentiation of Mycobacterium tuberculosis (Mtb) Complex to the Species Level by Utilizing High-Resolution Liquid Chromatography-Orbitrap™ Mass Spectrometry;** Suraj Saraswat¹; Amol O. Bajaj¹; Ping F. Yip²; Scott R. Kronewitter²; Adam P. Barker¹; ¹*ARUP Lab, Salt Lake City, UT*; ²*Thermo Fisher Scientific, Cambridge, MA*
- WP 668 **Rapid and Accurate Differentiation of Mycobacterium Abscessus Complex Isolates to the Species Level by High-Resolution Liquid Chromatography-Orbitrap™ Mass Spectrometry Assay;** Amol O. Bajaj¹; Suraj Saraswat¹; Ping F. Yip²; Scott R. Kronewitter²; Adam P. Barker¹; ¹*ARUP Laboratories, Salt Lake City, UT*; ²*Thermo Fisher Scientific, Cambridge, MA*
- WP 669 **Application of Multiplexed Ion Mobility MS for Identification of Host Response Protein Signatures of Treatment of Pulmonary Tuberculosis;** Komal Kedia¹; Jason Wendler¹; Erin S. Baker¹; Aaron T. Wright¹; Paul D. Piehowski¹; Marina A. Gritsenko¹; Richard D. Smith¹; Leah G. Jarsberg²; David M. Lewinsohn³; Marc H. Weiner⁴; Payam Nahid²; Jon M. Jacobs¹; ¹*PNPL, Richland, WA*; ²*UCSF, San Francisco, CA*; ³*Oregon Health & Science University, Portland, OR*; ⁴*University of Texas Health Science Center, San Antonio, TX*
- WP 670 **Time-resolved Global and Chromatin Proteomics during Herpes Simplex Virus (HSV-1) Infection;** Katarzyna Kulej^{1,2}; Daphne C. Avgousti^{1,2}; Simone Sidoli³; ⁴; Christin Herrmann^{2,5}; Ashley N. Della Fera²; Eui Tae Kim^{1,2}; Benjamin A. Garcia^{3,4}; Matthew D. Weitzman^{1,2}; ¹*Department of Pathology and Laboratory Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*; ²*Division of Cancer Pathobiology, Children's Hospital of Philadelphia, Philadelphia, PA*; ³*Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*; ⁴*Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*; ⁵*Cell and Molecular Biology Graduate Group, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*
- WP 671 **Toward Detection of Toxoplasmosis Reactivation from Urine Using Hydro-Gel Nanoparticles and Parallel Reaction Monitoring on an Orbitrap Fusion Mass Spectrometer;** Paul Russo¹; Hannah Steinberg²; Alessandra Luchini¹; Emanuel Petricoin¹; Lance Liotta¹; Robert H. Gilman²; Toxoplasmosis Working Group Universidad Peruana Cayetano Heredia³; ¹*George Mason University, Manassas, VA*; ²*Johns Hopkins University, Baltimore, MD*; ³*Toxoplasmosis Working Group at Universidad Peruana Cayetano Heredia, Lima, Peru*
- WP 672 **The DNA Sensor IFI1 Suppresses Viral Gene Transcription during HSV-1 Infection and is Counteracted by Virus-Induced Proteasomal Degradation;** Marni Crowl¹; Ileana Cristea¹; ¹*Princeton University, Princeton, NJ*
- WP 673 **Deciphering Human Sirtuin 3 Antiviral Functions and its Dynamic Regulation of the Mitochondria Acetylome during Infection;** Xinlei Sheng; ¹*Princeton University, Princeton, NJ*
- WP 674 **A Chemical Proteomic Strategy to unravel the Infectious Zika Virus Entry into Host Cells;** Mayank Srivastava¹; Andrew Miller¹; Yuan Zhou¹; Richard Kuhn¹; Andy Tao¹; ¹*Purdue University, West Lafayette*
- WP 675 **Putative Antimicrobial Peptides in the Lobster, Homarus americanus: Identification Using Top-Down and Bottom-Up Proteomics Coupled with Transcriptomics;** Daniel Do¹; Giap H. Vu¹; Patsy S. Dickinson¹; Andrew E. Christie²; Elizabeth A. Stemmler¹; ¹*Bowdoin College, Brunswick , ME*; ²*University of Hawaii at Manoa, Honolulu, Hawaii*
- WP 676 **Divergent and Coordinated Immune-Regulatory Roles of the Viral DNA Sensors IFI16 and cGAS during Viral Infection;** Krystal K Lum¹; Benjamin A. Diner¹; Bokai Song¹; Ileana M. Cristea¹; ¹*Princeton University, Princeton, NJ*

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- WP 677 **Nucleotide Ligand Binding and Exchange in Recombinant KRAS Using Native Mass Spectrometry;** Hemanth Akkiraju¹; Anna Kaplan¹; Lewis M. Brown¹; Brent R. Stockwell¹; ¹*Columbia University, New York , NY*
- WP 678 **Separation and Identification of Mouse Brain Microproteins using Top-down Method with High Resolution Nanocapillary Liquid Chromatography Mass Spectrometry;** Wenxue Li¹; Filomena Petruzzello¹; Nan



Zhao²; Huiyuan Zhao²; Xueting Ye²; Xiaozhe Zhang²; Gregor Rainer¹; ¹University of Fribourg, Fribourg, Switzerland; ²Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

WP 679 **Quantification of Proteoforms and Construction of Proteoform Families**; Michael R. Shortreed¹; Anthony J. Cesnik²; Brian L. Frey²; Leah V. Schaffer²; Rachel A. Knoener²; Mark Scalf²; Lloyd M. Smith²; ¹University of Wisconsin, Madison, WI; ²University of Wisconsin, Madison, WI

WP 680 **Method Development for Comprehensive Two Dimensional Liquid Chromatographic Separation and Triple Quadrupole Mass Spectrometric Quantitation of Intact Proteins**; Dananjaya Kalu Appulage¹; Yehia Z. Baghdady¹; Evelyn H. Wang²; Jorge Smith²; Ty Kahler³; Kevin A. Schug¹; ¹University of Texas at Arlington, Arlington, TX; ²Shimadzu Scientific Instruments, Columbia, MD; ³Restek Corporation, Bellefonte, PA

WP 681 **High Sensitivity and Accurate Mass Analyses of Intact Human Endogenous Proteins Produced Innaïve CD4 Cells using Nano Flow LC-MS**; Jason X. Tang¹; Kyoung-soo Choi¹; Stuart Bright¹; Chetan Patel¹; ¹Eli Lilly & Company, Branchburg, NJ

WP 682 **Elucidating E. coli Proteoform Families Using a Global PTM Discovery Database and Intact-mass Proteomics**; Yunxiang Dai¹; Robert J. Millikin¹; Anthony J. Cesnik¹; Michael R. Shortreed¹; Mark Scalf¹; Brian L. Frey¹; Lloyd M. Smith¹; ¹University of Wisconsin-Madison, Madison, WI

WP 683 **Using Random Sampling Statistics to Model Protein Isotope Distributions**; Zachary Philip Gotlib¹; Peter T. A. Reilly²; ¹Washington State University, Pullman, WA; ²Washington State University, Pullman, WA

WP 684 **Evidence for Glycation/Glycosylation of Low Molecular Weight Gluten Polymer Subunits in Wheat Kernels**; Ray Bacala^{1,2}; Hélène Perreault²; Dave Hatcher¹; ¹Canadian Grain Commission, Winnipeg, MB; ²Department of Chemistry, University of Manitoba, Winnipeg, MB

WP 685 **High Resolution LC-ESI-MS of Intact Wheat High Molecular Weight Glutenin Subunits (HMWGS) Reveals Unexpected Heterogeneity**; Katherine Cordova¹; Ray Bacala¹; Dave Hatcher¹; ¹Canadian Grain Commission, Winnipeg, MB

WP 686 **Dynamic pH Junction Based Capillary Zone Electrophoresis-Mass Spectrometry with Half-a-Microliter Loading Capacity for Top-Down Intact Protein Characterization**; Eli McCool¹; Rachele Lubeckyj¹; Liangliang Sun¹; ¹Department of Chemistry, Michigan State University, East Lansing, MI

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WP 687 **Whole and Phosphoproteome Analysis of Epithelial to Mesenchymal Transition in ES Derived RPE**; Joseph Leo Mertz¹; Srinivas R. Sripathi¹; Xue Yang¹; David Clark¹; Lijun Chen¹; Noriko Esumi¹; Hui Zhang¹; Donald J. Zack¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD

WP 688 **Systematic Proteome Profiling by DIA-MS to Characterize Calorie Restriction-Induced Life Span Extension in Yeast**; Lindsay K. Pino¹; Matt Kaeberlein¹; Andrew N. Hoofnagle¹; William S. Noble¹; Michael J. MacCoss¹; ¹University of Washington, Department of Chemistry, Seattle, WA

WP 689 **Quantitative Temporal Proteomics Analysis of Murine Bone Marrow Macrophages and RAW264.7 Cells in Osteoclast Differentiation**; Andrew Ng¹; Chengjian Tu^{2,3}; Shichen Shen^{3,4}; Jun Li^{2,3}; Jun Qu^{2,3,4}; Shuying Yang⁵; ¹Department of Oral Biology, School of Dental Medicine, University at Buffalo, State University of New York, Buffalo, NY; ²Department of Pharmaceutical Sciences, University at Buffalo, State University of New York, Buffalo, NY; ³New

York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, NY; ⁴Department of Biochemistry, School of Medicine and Biomedical Sciences, University at Buffalo, State University of New York, Buffalo, NY; ⁵Department of Anatomy and Cell Biology, School of Dental Medicine, University of Pennsylvania, Philadelphia, PA

WP 690 **Quantitative Proteomics Analysis of Heat Shock Proteins Involved in Unfolded Protein Response in Glioblastoma Cell Lines Induced by Different Drugs**; Jose Cesar Rosa¹; Helen Julie Laure¹; Carolina Thome¹; Germano Ferreira¹; Suely K.N. Marie²; Sueli Oba Shinjo²; Clarice Izumi¹; ¹Medical School of Ribeirao Preto University of Sao Paulo, Ribeirao Preto, SP; ²Medical School of Sao Paulo University of Sao Paulo, Sao Paulo, Brazil

WP 691 **Quantitative Profiling of Snake Venom using TMT Protein Labeling and Top-Down Mass Spectrometry**; Dahang Yu¹; Zhe Wang¹; Hongyan Ma¹; Si Wu¹; ¹University of Oklahoma, Norman, OK

WP 692 **Quantification of Metabolic Enzymes in the IDH1/2 Metabolic Pathways of Glioma Tissue using PRM**; Lennard J.M. Dekker¹; Suying Wu¹; Johan M. Kros¹; Dana Mustafa¹; Theo M. Luider¹; ¹Erasmus Medical Center, Rotterdam, Zuid Holland

WP 693 **Temporal Transcriptomic and Proteomic Landscapes of Pancreatic Islets in Type 2 Diabetic Rats**; Junjie Hou¹; Zonghong Li²; Wen Zhong³; Qiang Hao¹; Dongyu Zhao¹; Lei Lei¹; Linlin Wang¹; Pingyong Xu¹; Yifa Zhou²; You Wang¹; Tao Xu¹; ¹Institute of Biophysics, CAS, Beijing, China; ²Northeast Normal University, Changchun, China; ³HuaZhong University of Science and Technology, Wuhan, China

WP 694 **Enhanced Analysis of Host Cell Proteins from CHO cell cultured mAb using LC/MS**; Linfeng Wu¹; Jordy J. Hsiao¹; Te-Wei Chu¹; Pat Perkins¹; ¹Agilent Technologies, Santa Clara, CA

WP 695 **Targeted Quantification of Protein Phosphorylation in the Epidermal Growth Factor Receptor Signaling Pathway**; Lian Yi¹; Tujin Shi²; Fillmore L. Thomas²; Marina A. Gritsenko²; Yuqian Gao²; Tao Liu²; Richard D. Smith²; Steven H. Wiley²; Wei-Jun Qian²; ¹, Richland, WA; ²PNNL, Richland, WA

WP 696 **Organ-Level Proteomics of Systemic Infection Illuminates Dynamic Responses in a Mouse Model**; John Lapek¹; Robert Mills¹; Ronnie Fang¹; Brian Luk¹; Liangfang Zhang¹; Rob Knight¹; David Gonzalez¹; ¹UCSD, La Jolla, CA

WP 697 **Quantitative Proteomic Approach Reveals Landscape of the Regulatory Elements for Lysine-β-hydroxybutyrylation Pathway**; He Huang¹; Di Zhang¹; Yingming Zhao¹; ¹University of Chicago, Chicago, IL

WP 698 **Quantitative Multi-omics Characterization of Gemcitabine-induced Apoptosis and Resistance in Human Pancreatic Cancer Cells**; Xiaofang Zhong¹; Ling Hao¹; Jillian Johnson¹; Dustin Frost¹; Amanda Buchberger¹; John Kao²; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI; ²Hong Kong University of Science and Technology, Hong Kong, China

WP 699 **Characterizing Signaling Networks Associated with AMPK Activation in Human Myotubes by Isobaric Chemical Labeling Quantitative Phosphoproteomics**; Chuong Nguyen¹; Maryann Whitley²; Russell Miller²; Kimberly Cameron²; Ravi Kurumbail³; Kieran Geoghegan³; ¹Pfizer, Groton, CT; ²Pfizer, Cambridge, MA; ³Pfizer, Groton, CT

WP 700 **Quantitative Proteomic Analysis of Glucose Fasting Prior to Tandem Anti-Autophagy and Chemotherapy Treatment in Colorectal Cancer**; Monica Schroll¹; Gabriel LaBonia¹; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN

WP 701 **3D Imaging and Quantitative Proteomic Characterization of Bladder Stones and their Matrix Investigating a Cystinuria Mouse Model**; Tiffany Zee¹;



- WP 702 **Functional Consequences of Mutations in the Mammalian Target of Rapamycin Signaling Cascade;** Cassandra Wong^{1,2}; Geoffrey Hesketh¹; Anne-Claude Gingras^{1,2}; ¹Lunenfeld-Tanenbaum Research Institute, Toronto, ON, Canada; ²Department of Molecular Genetics, University of Toronto, Toronto, ON, Canada
- WP 703 **Quantitative Proteomics in a Non-Sequenced Vole Model: Insights into the Role of Brown Adipose Tissue Against Obesity;** Margaux Benhaim-Delarbre¹; Barbara Henning²; Georg Tascher¹; Pierre Bize³; Fabrice Bertile¹; ¹Institut Pluridisciplinaire Hubert Curien, CNRS, LMBIO, Université de Strasbourg, Strasbourg, France; ²Brazilian Institute of Neuroscience and Neurotechnology (BRAINN), University of Campinas, Brazil, Campinas, Brazil; ³Institute of Biological and Environmental Sciences, University of Aberdeen, Aberdeen, UK
- WP 704 **Gender-Specific Protein Expression of Lymphoblasts using Label Free LC/MS/MS;** Kathleen C Lundberg¹; Nicholas Szoko²; Daniela M Schlatter³; Marvin R Natowicz²; ¹Case Western Reserve University, Cleveland, OH; ²Cleveland Clinic Foundation, Cleveland, Ohio; ³Case Western Reserve University, Cleveland, OH
- WP 705 **Proteomic Storage Study of Probiotics;** Barbara S. Larsen¹; Ron Agee²; Michael Dauner³; Kurt Fenster²; Chris Hollard²; Cathy Kalbach³; Sunny Li³; Buffy Stahl²; Tom Mower³; Alexander Kopatsis³; Corban Rivera³; ¹The DuPont Company, Wilmington, DE; ²DuPont, Madison, WI; ³DuPont, Wilmington, DE
- WP 706 **A Mass Spectrometry-Based Proteomic Method to Discover RNA Binding Protein Complexes in Developing Rice Seeds;** Youngwoo Lee¹; Zach McBride¹; Daniel Szymanski¹; ¹Purdue University, West Lafayette, IN
- SYSTEMS BIOLOGY II**
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- WP 707 **An Unbiased Protein Association Study on the Public Human Proteome Reveals Biological Connections between Co-Occurring Protein Pairs;** Surya Gupta^{1,2,3}; Kenneth Verheggen^{1,2,3}; Jan Tavernier^{1,3}; Lennart Martens^{1,2,3}; ¹Department of Biochemistry, Ghent University, Ghent, Belgium; ²Bioinformatics Institute Ghent, Ghent University, Ghent, Belgium; ³Vib-Ugent Center For Medical Biotechnology, Ghent, Belgium
- WP 708 **Proteomic Analysis Reveals Novel Hydroxyproline-Dependent Cellular Pathways in Cancer Cells;** Luke Erber¹; Tong Zhou²; Yue Chen²; ¹University of Minnesota, Minneapolis, MN; ²University of Minnesota, Minneapolis, MN
- WP 709 **High pH Fractionation for Enhancing the Proteome Coverage in Tissues Dissected from the Early Frog (*Xenopus laevis*) Embryo;** Aparna B. Baxi^{1,2}; Camille Lombard-Banek¹; Sally A. Moody²; Peter Nemes¹; ¹Department of Chemistry, The George Washington University, Washington, D.C.; ²Department of Anatomy & Regenerative Biology, The George Washington University, Washington, D.C.
- WP 710 **Multi-Omics Comparative Analysis Reveals Host Signaling Pathways Affected by the Gut Microbiota;** Nathan P Manes¹; Natalia Shulzhenko²; Arthur G Nuccio¹; Sara Azeem¹; Andrey Morgun²; Aleksandra Nita-Lazar¹; ¹National Institutes of Health, Bethesda, MD; ²Oregon State University, Corvallis, OR
- WP 711 **A Multiproteomic Approach to Characterize Transcriptional Regulators of HIV Expression During Activation of Primary CD4+T Cell Hosts;** Mei Leng¹; Alexander Saltzman¹; Bhoomi Bhatt¹; Anna Malovannaya¹; ¹Baylor College of Medicine, Houston, TX
- WP 712 **In-depth Analyses of Protein Abundance, Phosphorylation, Synthesis and Degradation during Neuronal Development and Synaptic Plasticity;** Renske Penning¹; Christian K. Frese¹; Charlotte A.G.H. van Gelder¹; Marina Mikhaylova¹; Riccardo Stucchi¹; Harm Post¹; Albert J. R. Heck¹; Harold D. MacGillavry¹; Casper C. Hoogenraad¹; A.F. Maarten Altelaar²; ¹Utrecht University, Utrecht, Netherlands; ²Utrecht University, Utrecht
- WP 713 **Quantitative Proteomics and Immunohistochemistry Reveal Insights into Cellular and Molecular Processes in the Infarct Border Zone after Myocardial Infarction;** Zachery R Gregorich¹; Libang Yang²; Wenxuan Cai³; Patrick Zhang²; Bernice Young²; Yiwen Gu³; Jianyi Zhang⁴; Ying Ge³; ¹UW Madison, Madison, WI; ²University of Minnesota, Minneapolis, MN; ³University of Wisconsin Madison, Madison, WI; ⁴University of Alabama at Birmingham, Birmingham, AL
- WP 714 **Pathway Visualization and Analysis for Quantitative Posttranslational Modification and Proteome Time Series Data in the Perseus Software;** Jan Rudolph¹; Stefka Tyanova²; John C. Rogers³; Bhavin Patel³; Shouling Xu^{4,5}; Devin Drew⁶; Kai Fritzemeier⁶; Andreas F. Huhmer⁷; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Hoffmann-La Roche, Basel, Switzerland; ³Thermo Fisher Scientific, Rockford, IL; ⁴Stanford University School of Medicine, Palo Alto, CA; ⁵Thermo Fisher Scientific, San Jose, CA; ⁶Thermo Fisher Scientific, Bremen, Germany; ⁷Thermo Fisher, San Jose, CA
- WP 715 **Analysis of Neonatal Mouse Hearts with Shotgun Proteomics and Untargeted Metabolomics;** Päivi Pöhö¹; Jaakko Teppo^{1,2}; Virpi Talman³; Anu Vaikkinen¹; Sini Kinnunen³; Kajetan Trost⁴; Tommi Suviola⁴; Peter Rossing⁴; Tapio Kotiaho^{1,5}; Heikki Ruskoaho³; Markku Varjosalo²; Risto Kostinen¹; ¹Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland; ²Molecular Systems Biology Research Group and Proteomics Unit, Institute of Biotechnology, University of Helsinki, Helsinki, Finland; ³Division of Pharmacology and Pharmacotherapy, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland; ⁴Steno Diabetes Center Copenhagen, Gentofte, Denmark; ⁵Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland
- WP 716 **Broad-scale Proteomic Analysis of Subcellular Fractions for the High-Throughput Investigation of Mechanism of Action;** Danielle B. Gutierrez¹; Melissa A. Farrow²; Carrie E. Romer¹; Jamie L. Allen¹; Yuan-wei Nei¹; Jocelyn Simpson²; Tina Tsui¹; Salisha Hill¹; Kristie L. Rose¹; Jeremy L. Norris¹; D. Borden Lacy²; Eric P. Skaar²; Richard M. Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²Vanderbilt University Medical Center, Nashville, TN
- WP 717 **Quantitative Multidimensional Characterization of Protein-Protein Interactions in Cancer;** Danielle Swaney¹; Margaret Soucheray¹; Nevan Krogan¹; ¹UCSF, San Francisco, CA
- WP 718 **REPRINT: A Resource for Evaluation of Protein Interaction Networks;** Dattatreya Mellacheruvu¹; Zachary Wright¹; Felipe da Veiga Leprevost¹; Anne-Claude Gingras²; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI; ²Lunenfeld-Tanenbaum Research Institute, Toronto, ON, Canada
- WP 719 **Mapping Ubiquitin Regulation under Stress by Multi-Dimensional Proteomics;** Jeremy O'Connell¹; Marta Isasa²; Joao Paulo¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA; ²C4 Therapeutics, Cambridge, MA; ³Pharma Services, Inc., Lincolnshire, IL; ⁴Q2 Lab Solutions Bioanalytical and ADME Labs, Ithaca, NY; ⁵Quintiles, Ithaca, NY



THURSDAY POSTERS

Set up all Thursday posters7:30 – 8:00 am
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Even-numbered posters present 12:00 – 2:30 pm
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BIOMARKERS: DISCOVERY II 001 - 024

- ThP 001 **Biomarker Discovery in Fragile X-Associated Tremor/Ataxia Syndrome Using Mass Spectrometry Based Proteomics**; Amber Orcutt¹; Vadi Bhat²; Carol Haney-Ball²; Deborah A. Hall¹; Stephanie Cologna³; Elizabeth M. Berry-Kravis¹; ¹Rush University, Chicago, IL; ²Agilent Technologies, Wilmington, DE; ³University of Illinois at Chicago, Chicago, Illinois
- ThP 002 **Annexin A10 is a Candidate Marker Associated with the Progression of Pancreatic Precursor Lesions to Adenocarcinoma**; Jianhui Zhu¹; Jing Wu¹; Xiucong Pei¹; Zhijing Tan¹; Mingrui An¹; Jiaqi Shi¹; David M. Lubman¹; ¹University of Michigan Medical Center, Ann Arbor, MI
- ThP 003 **Cross-Panel Analysis of INLIGHT™ N-Linked Glycans in the Avian Model of Ovarian Cancer**; Elizabeth S. Hecht¹; Alison A. Motsinger-Reif¹; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC
- ThP 004 **Development of a Novel Chemical Method for Serum/Plasma Protein Depletion**; Anton Iliuk¹; Li Li¹; Keerthi Jayasundera²; Andy Tao^{1,2}; ¹Tymora Analytical Operations, West Lafayette, IN; ²Purdue University, West Lafayette, IN
- ThP 005 **Discovery of Exposure Markers of di(2-pro,pylheptyl) phthalate (DHPH) Using Mass Spectrometry and Two Data Screening Procedures**; Pao-Chi Liao¹; Chia-Lung Shih¹; Pao-Mei Liao²; Jen-Yi Hsu¹; ¹Department

of Environmental and Occupational Health, College of Medicine, National Cheng Kung University, Tainan, Taiwan; ²Department of Environmental Science and Property Management, Jinwen University of Science and Technology, New Taipei City, Taiwan

- ThP 006 **Identification of Hypoxia-Induced Splicing Variants in Cancer Cells Using Proteomics Approach**; Pang-Hung Hsu¹; Chia-Hung Li¹; ¹National Taiwan Ocean University, Keelung, Taiwan
- ThP 007 **Morphology Mass Spectrometry Imaging to Discover Heterogeneity Markers in Oncology**; Gael Picard de Muller¹; Rima Ait-Belkacem¹; Fabien Pamelard¹; David Bonnel¹; Jonathan Stauber¹; ¹Imabiotech, Loos, France
- ThP 008 **Identification of Cerebrospinal Fluid Peptide Markers for Recurrent Malignant Brain Tumor by Quantitative Proteomics**; Tomohiro Kohata¹; Shingo Ito¹; Kumamoto, Japan; Mio Hirayama¹; Kumamoto, Japan; Takuya Furuta¹; Kanazawa, Japan; Mitsutoshi Nakada¹; Kanazawa, Japan; Sumio Ohtsuki¹; Kumamoto, Japan
- ThP 009 **Screening of Diabetes Mellitus, Colorectal Cancer Complicated with Diabetes and Colorectal Cancer by Simultaneous Targeted and Non-Targeted Quantitative Metabolomics Analysis**; Yang Gao¹; Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, China
- ThP 010 **Parkinson's Disease Cerebral Spinal Fluid Analysis by Direct Injection Electrosonic Spray Ionization Multiple Reaction Monitoring-Profiling**; Karen E. Yannell¹; Christina R. Ferreira²; Tiago JP Sobreira²; R. Graham Cooks²; ¹Purdue University, west lafayette, IN - Indiana; ²Purdue University, West lafayette, Indiana
- ThP 011 **Comprehensive, Unbiased Proteomic Profiling of the Cell-Surface, Exosomal, and Secreted Proteomes of Senescent Cells**; Natan Basisty¹; Bradford W Gibson¹; Judith Campisi¹; Birgit Schilling¹; ¹The Buck Institute for Research on Aging, Novato, CA
- ThP 012 **Quantification of *in vivo* Protein Molecular Dynamics Employing Stable Isotope Labeling with Deuterium Oxide and High Resolution Mass Spectrometry**; Thomas E Angel¹; Matthew E Szapacs¹; Zhuo Chen¹; Christopher A Evans¹; ¹GSK, King of Prussia, PA
- ThP 013 **Proteomic Analyses of GNMT Knock-Out Mice – the Translational Research Study of mARC Genes Related to Liver Cancer**; Ming-Hui Yang¹; Yi-Ming Arthur Chen¹; Hsiao-Hsuan Mo¹; Yu-Chang Tyan¹; ¹Kaohsiung Medical University, Kaohsiung, Taiwan
- ThP 014 **Identification and Label-Free Quantification of Lipid Based Markers for Pre-Term Birth Using a Novel Scanning Quadrupole DIA Acquisition Method**; Lee A Gethings¹; Shirish Yakkundi²; Gregoire Thomas³; Aude-Clare Morillon²; James I Langridge¹; Louise Kenny²; ¹Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; ²INFANT, Cork, Ireland; ³Squ4re, Wevelgem, Belgium
- ThP 015 **Determination of Metabolomics Profile Changes for Prediction of Mortality in Induced Hypothermia after Cardiac Arrest Patients**; Urszula Osinska Warncke¹; Mary Ann Peberdy¹; Dayanjan S Wijesinghe¹; ¹Virginia Commonwealth University, Richmond, Virginia
- ThP 016 **Deepest Plasma Proteome Coverage with Lumos**; Yue Zhou¹; Aiying Nie²; Jing Li¹; ¹ThermoFisher Scientific, Shanghai, China; ²ThermoFisher Scientific, shanghai, China
- ThP 017 **Discovery and Characterization of Leukemia Chemotherapy-Related Neurotoxicity Biomarkers in Cerebrospinal Fluid via Mass Spectrometry-based Shotgun Proteomics**; Qinying Yu¹; Bingming Chen¹; Yu Feng¹; Chrysanthi Ikonomidou¹; Lingjun Li¹; ¹University of Wisconsin Madison, Madison, WI
- ThP 018 **Probing Exosomes for Early-Stage Biomarkers of Coronary Artery Disease**; Sarah Elder¹; Blair Chen¹; Weiguo Andy Tao¹; ¹Purdue, West Lafayette, IN



- ThP 019 **Optimizing Differential Ion Mobility-Mass Spectrometry based Leukemia Antigen Detection;** Ian M Schlup¹; James E Keating¹; Sally Hunsucker²; Courtney Elliot²; Paul Armistead²; Gary L Glish¹; ¹University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC; ²Lineberger Comprehensive Cancer Center, Chapel Hill, NC
- ThP 020 **Identification, Validation and Quantification of Neuregulin-4 by Immunoreactive Methods in Blood Samples from Patients With or Without Diabetes;** Rong-Ming Lyu¹; Nae J Dun²; Xianghai Yao¹; Qing Tian¹; Siok Le Dun²; Jin Jun Luo²; Jaw-Kang Chang¹; ¹Phoenix Pharmaceuticals, Burlingame, CA; ²Temple University, Philadelphia, PA 19140
- ThP 021 **Analysis of Cellular and Exosomal Proteins to Decode LKB1 Regulated Pathways in Lung Cancer Invasion and Metastasis;** Bernice Agana¹; Michael Koenig²; Takehito Shukuya²; Joseph Amann²; David Carbone²; Vicki Wysocki¹; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Department of Internal Medicine, The Ohio State University, Columbus, OH
- ThP 022 **MIK-MS (Molecular Interaction and Kinetics Mass Spectrometry) Used to Verify the Affinity Ranking of Protein-Small Molecule Interactions;** Tetsuya Fukuda¹; Naoko Ohi²; Noboru Nakayama³; John Ervin⁴; Yasuhiko Bando¹; Toshihide Nishimura³; Toshiaki Somehara²; Satoru Nagatoishi⁵; Kouhei Tsumoto⁶; Takeshi Kawamura⁷; ¹Research and Development, Biosys Technologies, Inc., Meguro-ku, Japan; ²Research & Marketing, Nissha Printing Co., Ltd., Kyoto-shi, Japan; ³Translational Medicine Informatics, St. Marianna University School of Medicine, Kawasaki-shi, Japan; ⁴Silicon Kinetics, Inc., San Diego, CA; ⁵School of Engineering, The University of Tokyo, Minato-ku, Japan; ⁶School of Engineering, The Institute of Medical Science, and Drug Discovery Initiative, The University of Tokyo, Minato-ku, Japan; ⁷Proteomics Laboratory, Radioisotope Center, The University of Tokyo, Bunkyo-ku, Japan
- ThP 023 **Methods in Purity Optimization for A1AT Glycopeptide Analysis in Biomarker Research;** Elisa Warner¹; Jianhui Zhu²; David M. Lubman²; ¹Ann Arbor, MI; ²University of Michigan Medical School, Ann Arbor, MI
- ThP 024 **Identification of Single Amino Acid Variants from Three Subpopulations in the MCF-7 Breast Cancer Cell Line;** Zhijing Tan¹; Song Nie^{1,2}; Sean P. McDermott¹; Max S. Wicha¹; David M. Lubman¹; ¹The University of Michigan, Ann Arbor, MI; ²Pacific Northwest National Laboratory, Richland, WA
- BIOMARKERS: QUANTITATIVE ANALYSIS III**
025 - 051
- ThP 025 **Using SRM to Monitor Biomarkers for Clostridium Difficile Susceptibility;** Sigmund J Haidacher^{1,2}; Kathleen M Hoch^{1,2}; Prapaporn Boonma^{2,3}; Jennifer M Auchtung³; Robert A Britton³; Tor Savidge^{2,3}; Anthony M Haag^{2,3}; ¹Baylor College of Medicine, Houston, TX; ²Texas Children's Hospital, Houston, TX; ³Baylor College of Medicine, Houston, TX
- ThP 026 **Function of Human Gut Microbiome in Chronic Kidney Disease: Metaproteomics Approach;** Oleg K Karaduta¹; Gerren P Hobby¹; Galina V Glazko¹; Yasir Rahmatallah¹; Lisa M Orr¹; Samuel G Mackintosh¹; Ricky D Edmondson¹; John M Arthur¹; Boris L Zybailov¹; ¹UAMS, Little Rock, AR
- ThP 027 **Pre-Analytical Variability Assessment for Human Plasma Samples Based on Inflammation Biomarkers and Abundant Proteins;** Zhijun Cao¹; Jinchun Sun¹; Laura Schnackenberg¹; Lisa Pence¹; Tom Schmitt¹; Mackean Maisha¹; Antje Wagner-Golbs²; Beate Kamlage²; Richard D Beger³; Li-Rong Yu¹; ¹National Center for Toxicological Research, FDA, Jefferson, AR; ²Metanomics GmbH, Berlin, Germany; ³NCTR/FDA, Jefferson, AR
- ThP 028 **Don't Know Activity from ADAM(TS13)? The First LC-MS/MS Assay for Measuring Activity of von Willebrand Factor Cleaving Protease;** Meghan Bradley¹; Russell Grant¹; Christopher M Shuford¹; ¹LabCorp, Burlington, NC
- ThP 029 **Quantification of Bile Acids and their Conjugates in Plasma by Liquid Chromatography/Full Scan High Resolution Mass Spectrometry;** Yao Shi¹; Michael Van Parys¹; Yang Gao¹; Dennis Milanowski¹; Stephanie Cape¹; Xiaorong Liang²; Brian Dean²; ¹Covance, Madison, WI 53704; ²Genentech, Inc, South San Francisco, CA
- ThP 030 **Sensitive and Reproducible LC-MS Quantification of C-Reactive Protein in Plasma Using a Generic Kit-Based Approach for Clinical Research;** Paula Orens¹; Mary E Lame²; Steven Calciano²; Erin Chambers²; ¹Waters Corporation, Milford, MA; ²Waters Corp, Milford, MA
- ThP 031 **Glycoproteomics of Breast Cancer Human Plasma Extracellular Vesicles for Biomarker Discovery and Validation Using Polymer-Based Reverse Phase Glycoprotein Array;** Hillary Andaluz¹; I-Hsuan Chen¹; Li Pan¹; Anton Iliuk^{1,2}; Andy Tao^{1,2}; ¹Purdue University, West Lafayette, Indiana; ²Tymora Analytical Operations, West Lafayette, IN
- ThP 032 **LC/MS Analysis of Various Compounds Having Amino or Ammonium Groups with Using a New Polymer-based HILIC Column;** Junji Sasuga¹; Daisuke Maruyama¹; Ron Benson²; Leah Block²; ¹Showa Denko KK, Ogimachi, Japan; ²Shodex, Showa Denko America, Inc., New York, NY
- ThP 033 **A Simple Dilute-and-Shoot FI-MS/MS for Quantification of Glycocholic Acid in Human Bile Using Standard Addition Method;** Raghavi Kakarla¹; Ramakrishna Reddy Voggu¹; Baochuan Guo²; Janet Donaldson³; ¹Cleveland State University, Cleveland, OH; ²Cleveland State University, Department of Chemistry, Cleveland, OH; ³Mississippi State University, Starkville, MS
- ThP 034 **Quantitative MALDI-TOF Measurements of Protein Functional Activity in Bronchoalveolar Lavage and Serum for Rapid Adverse Drug Reactions Assessment;** Ilya Toropygin¹; Alexandr Protasov²; Olga Mirgorodskaya²; Andry Vasin²; Andrey Lisitsa¹; ¹Inst. of Biomedical Chemistry, Moscow, Moscow; ²Research Institute of Influenza, Saint-Petersburg, Russia
- ThP 035 **Quantitation of a Broad Range of Nucleotides in Mouse Tissues Using a Novel Liquid Chromatography/Mass Spectrometry Method;** Chris Petucci^{1,2}; Andrew Zelenin^{2,3}; Nidhi Kapoor^{2,3}; Meghan Gabriel^{2,3}; Mauro Dispagna^{2,3}; Stephen J. Gardell^{2,3}; ¹Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; ²University of Florida, Gainesville, FL; ³Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL
- ThP 036 **Detection and Quantification of Bufadienolides in Complex Sample Mixtures Using a nano-ESI-IM-MS Coupled to nano-UPLC;** Luke T. Richardson¹; Brooke A. Brown¹; Elyssia S Gallagher¹; Jules B. Puschett²; Touradj Solouki¹; ¹Baylor University, Waco, Texas; ²Texas A&M University, College Station, Texas
- ThP 037 **Urinary Metabolomics and Proteomics Analysis of an E.coli-Induced Prostatic Inflammation Mouse Model via Isobaric DiLeu Tagging and Label-free Methods;** Pingli Wei¹; Ling Hao²; Fengfei Ma³; Qing Yu³; Amanda Buchberger⁴; Sanghee Lee⁵; Wade Bushman⁵; Lingjun Li^{1,3}; ¹Department of chemistry, University of Wisconsin Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³School of pharmacy, University of Wisconsin Madison, Madison, WI; ⁴Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ⁵Department of Urology, University of Wisconsin-Madison, Madison, WI
- ThP 038 **Imputation of Missing Data in Quantitative Proteomics using Singular Value Thresholding;** Tjeerd Dijkstra¹; Timo Sachsenberg²; Oliver Kohlbacher³; ¹Max Planck Institute for



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- Developmental Biology, Tuebingen, Germany; ²Universität Tübingen, Tübingen, Germany; ³Max Planck Institute for Developmental Biology, Tübingen, Germany
- ThP 039 **Ultra-Trace Level Quantitation of Modified Human Lung DNA: Extreme Efforts to Optimize the Sensitivity of HRAM Detection of Adducted Nucleosides**; J. Bradley Hochalter¹; Peter W. Villalta¹; Stephen S. Hecht¹; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN
- ThP 040 **Selective Enrichment of Biomarkers Using Amphiphilic Polymers for Enhanced Mass Spectrometric Analysis**; Mahalia A. C. Serrano¹; Bo Zhao¹; Sankaran Thayumanavan¹; Richard W Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- ThP 041 **Protein Biomarker Discovery for Patient with Gastric Cancer Using Mass Spectrometry-Based Quantitative Urinary Proteomics**; Hong Wang¹; Hiroaki Katayama¹; Xiaoqian Liu¹; Juan Chen¹; Ayumu Taguchi¹; Samir Hanash¹; ¹MD Anderson Cancer Center, Houston, TX
- ThP 042 **The Experimental Autoimmune Myocarditis in Rat Activates the Autophagy and Apoptosis**; Jong Bok Seo¹; Seung-Min Choi¹; ¹Korea Basic Science Institute, Seoul, Asia
- ThP 043 **A Quantitative Analytical Method for PIVKA-II Using Multiple Reaction Monitoring-Mass Spectrometry for Early Diagnosis of Hepatocellular Carcinoma**; Areum Sohn¹; Hyunsoo Kim²; Dongyoon Shin³; Youngsoo Kim^{1,4}; ¹Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea; ²Seoul National University Hospital, Seoul, Jongro-gu; ³Seoul National University College of Medicine, Seoul, South Korea; ⁴Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Seoul, South Korea, Seoul, South Korea
- ThP 044 **Development and Qualification of a Sensitive and Robust Immunoaffinity UPLC-MRM MS Method for Quantitative Measurement of Angiopoietin-1 in Monkey Plasma**; Yuhuan Ji¹; Joshuaine Toth²; Tammy Bigwarfe²; Chao Zheng²; Margit MacDougall²; Qian Li¹; Jian Shi¹; Vladimir Papov²; Peng Sun²; Ryan Fryer²; John Chen¹; Laixin wang¹; Chengjie Ji¹; ¹Novabioassays LLC, Woburn, MA; ²Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT
- ThP 045 **Measuring Microbial Load in Unburned Tobacco using HPLC and Tandem Mass spectrometry**; Peter Kuklennyik¹; Jacob B. Kimbrell^{1,2}; Robert Tyx¹; Angel J. Rivera^{1,2}; Stephen Stanfill¹; ¹Centers for Disease Control, Atlanta, Georgia; ²Oak Ridge Institute of Science & Education, WPAFB, OH
- ThP 046 **Streamlining Quantitative Assay Development Using Diagnostic Cluster Ions Native to Atmospheric Pressure Ionization**; RICHARD KING¹; Susan Crathern¹; Guille Metzler¹; Lorin Bachmann²; carmen fernandez-metzler¹; ¹PharmaCadence Analytical Services, LLC, Hatfield, PA; ²Virginia Commonwealth University, Richmond, VA
- ThP 047 **Development of a nonglycopeptide-based MRM strategy for screening of differential glycoproteins in hepatocellular carcinoma**; Weiqian Cao¹; Bingyun Jiang²; Jiangming Huang²; Yi Wang²; Pengyuan Yang²; ¹Fudan University, Shanghai, Shanghai; ²Fudan University, Shanghai, China
- ThP 048 **Epitope fishing in digested biological samples**; Maren Levernaes¹; Bassem Farhat¹; Marianne Nordlund Broughton²; Léon Reubsæt¹; Trine Grønhaug Halvorsen¹; ¹School of Pharmacy, University of Oslo, Oslo, Norway; ²Department of Medical Biochemistry, Radiumhospitalet, Oslo University Hospital, Oslo, Norway
- ThP 049 **Comparison of Short-Chain Fatty Acids in Fecal vs. Plasma Samples using Gas Chromatography-Mass Spectrometry as Markers for the Gut Microbiome**; Vincent Windisch¹; John A. Masucci²; Allen Xu¹; ¹Keystone Bioanalytical, North Wales, PA; ²Janssen Research&Development, Spring House, PA
- ThP 050 **Highly Sensitive Mass Spectrometric Analysis of Tau Protein Isoforms in Human Cerebrospinal Fluid**; Yusaku Hioki¹; Naoki Kaneko¹; Ritsuko Yoda¹; Sadanori Sekiya¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 051 **MRM based Validation of Protein Biomarkers across Different Grades of Glioma Tissues**; Nikita Gahoi¹; Saicharan Ghantasala¹; Kishore Gollapalli¹; Sanjeeva Srivastava¹; Ajit Datar²; Rashmi Kochhar²; Aliasgar Moiyadi³; Epari Sridhar³; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ³Tata Memorial Hospital, Parel, Mumbai, India
- ### BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING II
- #### 052 - 072
- ThP 052 **Improving Mass-Spectrometry Analysis of Protein Structures with Arginine-Specific Chemical Cross-linkers**; Alexander X. Jones¹; Yong Cao²; Yue-He Ding²; Hui Tan¹; Meng-Qiu Dong²; Xiaoguang Lei¹; ¹College of Chemistry, Peking University, Beijing, China; ²National Institute of Biological Sciences, Beijing, Beijing, China
- ThP 053 **Optimization of Zero-Length Cross-linking Reaction Conditions Using Liquid Chromatography Mass Spectrometry to Probe Large Protein Complexes**; Pengyuan Liu¹; Yekaterina Kori¹; Sandra L. Harper¹; Roland Rivera-Santiago¹; David W. Speicher¹; ¹The Wistar Institute, Philadelphia, PA
- ThP 054 **de novo Protein Structure Determination by Short-Distance Crosslinking Constraint-Guided Discrete Molecular Dynamics Simulations**; Nicholas I. Brodie¹; Jason J. Serpa¹; Konstantin I. Popov²; Evgeniy V. Petrotchenko¹; Nikolay V. Dokholyan²; Christoph H. Borchers^{1,3}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochemistry and Biophysics, University of North Carolina School of Medicine, Chapel Hill, NC; ³Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- ThP 055 **Novel Photo-Reactive Homo-Bifunctional Bis-Diazirine Short-Range Crosslinkers for Studying Protein Structure**; Nicholas I. Brodie¹; Jason J. Serpa¹; Evgeniy V. Petrotchenko¹; Christoph H. Borchers^{1,2}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- ThP 056 **NSLS-II XFP: X-ray Footprinting Beamline for in vitro and in vivo Structural Studies of Biological Macromolecules**; Jen Bohon^{1,2}; Don Abel¹; Erik R. Farquhar¹; John Toomey¹; Michael Sullivan¹; Mark R. Chance^{1,2,3}; ¹Center for Synchrotron Biosciences, Case Western Reserve University, Cleveland, OH; ²Department of Nutrition, Case Western Reserve University, Cleveland, OH; ³Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH
- ThP 057 **Kojak: Pipeline Developments and New Features for the Analysis of Chemically Cross-Linked Proteins**; Michael R. Hoopmann¹; Alex Zelter²; Michael Riffle²; Luis Mendoza³; David Shteynberg¹; Eric W. Deutsch¹; Trisha N. Davis²; Robert L. Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of Washington, Seattle, WA
- ThP 058 **Evaluation of a Series of Arginine-Specific Chemical Cross-Linkers for Mass Spectrometry Analysis of Proteins**; Alexander X. Jones¹; Yong Cao²; Yue-He Ding²; Xiaoguang Lei¹; Meng-Qiu Dong²; ¹College of Chemistry, Peking University, Beijing, China; ²National Institute of Biological Sciences, Beijing, Beijing, China



- ThP 059 **Label-free Quantitative Cross-Linking for Conformational Analysis by SIM-XL**; Fabio C Gozzo¹; Luana Oliveira¹; Allan JR Ferrari¹; Diogo Borges Lima²; Paulo Costa Carvalho³; ¹University of Campinas, Campinas, SP; ²Institut Pasteur, Paris; ³Carlos Chagas Institute - Fiocruz, Curitiba, Brazil
- ThP 060 **OpenProXL: a Fast and Versatile XL-MS Identification Tool**; Eugen Netz¹; Timo Sachsenberg²; Christian Johannes Gloeckner³; Oliver Kohlbacher^{1,2}; ¹Max Planck Institute for Developmental Biology, Tübingen, Germany; ²Universität Tübingen, Tübingen, Germany; ³German Center for Neurodegenerative Diseases Tübingen, Tübingen, Germany
- ThP 061 **Hydroxyl Radical Footprinting with PLIMB (Plasma-Induced Modification of Biomolecules): A New Tool for Structural Mass Spectrometry**; Benjamin B. Minkoff¹; Joshua Blatz¹; Daniel Benjamin¹; Faraz Choudhury¹; J. Leon Shohet¹; Michael R. Sussman¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 062 **Fast Photochemical Oxidation of Proteins Coupled with Ion Mobility-Mass Spectrometry to Characterize Structural Differences between Protein Conformers**; Emily Hart¹; Daniel J. Deredge¹; Lisa M. Jones¹; ¹University of Maryland School of Pharmacy, Baltimore, MD
- ThP 063 **Perfluoroalkyl Radicals for Footprinting Soluble and Membrane Proteins**; Ming Cheng¹; Michael L. Gross²; ¹Washington University, St. Louis, MO; ²Washington University, St. Louis, MO
- ThP 064 **High Resolution Mapping of Drug Binding Site Using Hydroxyl Radical Footprinting**; Janna Kiseler¹; Stephanie Stanford^{2,3}; Alexander E Aleshin⁴; Sichun Yang¹; Vida Zhang^{2,3}; Robert J Ardecky⁵; Gregory W Cadwell⁴; Jinghua Yu⁵; Laurie A Bankston⁴; Robert C Liddington⁴; Anthony Pinkerton⁵; Mark R Cance¹; Nunzio Bottini^{2,3}; ¹Department of Nutrition, Case Western Reserve Univ, Cleveland, OH; ²Division of Cellular Biology, La Jolla Institute for Allergy and Immunology, La Jolla, CA; ³Department of Medicine, University of California, San Diego, CA; ⁴Infectious and Inflammatory Disease Center, Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA; ⁵Conrad Prebys Center for Chemical Genomics, Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA
- ThP 065 **Amino Acid Analysis of Carbene Footprinting by Enzymatic Hydrolysis and GC-MS**; Bojie Zhang¹; Daryl Giblin¹; Ming Cheng¹; Michael L. Gross¹; ¹Washington University in St. Louis, St. Louis, MO
- ThP 066 **Structural Elucidation via Automated Analysis of Complex Protein Crosslinking Data**; Allis S. Chien¹; Eric Carlson²; Marshall W. Bern²; Wilfred H. Tang²; Christopher Becker²; Ryan D. Leib¹; Christopher M. Adams¹; ¹Vincent Coates Foundation Mass Spectrometry Laboratory, Stanford University, Stanford, CA; ²Protein Metrics Inc., San Carlos, CA
- ThP 067 **High Confidence Identification of Crosslinked Peptides Using a Dual Cleavable Crosslinker (DUCCT) with Enrichment Functionality**; Jayanta Kishor Chakrabarty¹; Abu Hena M Kamal²; Zixiang Fang²; Saiful M. Chowdhury²; ¹University of Texas, Arlington, Arlington, TX; ²University of Texas at Arlington, Arlington, TX
- ThP 068 **Carbonate Radical Anion as a new reagent for Fast Photochemical Oxidation of Proteins**; Mengru Zhang¹; Michael L. Gross²; ¹St. Louis, Missouri; ²WUSTL, St. Louis, MO
- ThP 069 **Enrichment Strategies for Improvement of Mass Spec Analysis of Chemical Cross-Linked Peptides**; Rosa Viner¹; Ryan Bomgarden²; Kratika Singhal²; Sergei Snovidia²; Craig Gutierrez³; Lan Huang³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Rockford, IL; ³UC Irvine Department of Physiology & Biophysics, Irvine, CA
- ThP 070 **Chemical Cross-Linking (CXL) Products Analysed by LC-Ion Mobility (IM)-MS/MS**; Denise P Tran¹; Paul J Trim²; Marten F Snel²; Tara L Pukala¹; ¹The University of Adelaide, Adelaide, Australia; ²South Australian Health and Medical Research Institute, Adelaide, Australia
- ThP 071 **MS-Fold: Protein Structure Prediction Guided by Covalent Labeling Mass Spectrometry Data**; Melanie L Arahamian¹; Samantha H Hinckley¹; Vicki H. Wysocki¹; Steffen Lindert¹; ¹Ohio State University, Columbus, OH
- ThP 072 **Cross-Linking Visualization and Analysis Using CX-Circos 2**; Junjie Wang¹; Yi Shi¹; Brian T Chait¹; ¹Rockefeller University, New York, NY
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- ThP 073 **A High Sensitivity LC/MS/MS Method for Quantitative Analysis of Eight Antifungal Drugs in Human Serum**; Tze Peng Lim¹; Yuan Cao²; Shao Hua Chia²; Si Xuan Tan¹; Zhao Qi Zhan²; Jie Xing²; ¹Pharmacy, Singapore General Hospital, Singapore, Singapore; ²Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore, Singapore
- ThP 074 **Direct Injection of Antiretroviral Drugs in Highly Organic Protein-Precipitated Human Plasma by LC-MS/MS**; Frances Carroll¹; Justin Steimling¹; Susan Steinike¹; ¹Restek Corporation, Bellefonte, PA
- ThP 075 **Quantification of 3 α and 3 β epimers of 25-Hydroxyvitamin D3 in DBS Using Artificial Whole Blood Calibration and Chemical Derivatization**; Miriam Müller¹; Caroline Stokes¹; Dietrich Volmer¹; ¹Saarland University, Saarbrücken
- ThP 076 **LC-MS-MS Quantitative Analysis of Thyroid Hormones and Metabolites in Serum for Research Use**; Rory M. Doyle; Thermo Fisher Scientific, Somerset, NJ
- ThP 077 **Rapid Quantification of Endogenous Cholesterol in Human Serum on Filter Paper Using Direct Analysis in Real Time Mass Spectrometry (pDART-MS)**; Hua-Yi Hsieh¹; Li-Hua Li^{2,3}; Ren-Yu Hsu¹; Ying-Chen Huang¹; Wei-Fong Kao^{4,5}; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; ³School of Medical Laboratory Science and Biotechnology, Taipei Medical University, Taipei, Taiwan; ⁴Chief, Department of Emergency & Critical Care Medicine, Taipei Medical University Hospital, Taipei, Taiwan; ⁵Department of Emergency medicine, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan
- ThP 078 **Enzyme Activities in Six Lysosomal Storage Diseases in Japanese Neonates Determined by LC-MS/MS**; Ryuichi Mashima¹; Motomichi Kosuga¹; Torayuki Okuyama¹; ¹National Center for Child Health and Development, Setagaya-ku, Japan
- ThP 079 **Quantitative Analysis of β -Lactam Antibiotics in Human Plasma by High Sensitivity LC/MS/MS Method**; Daryl Kim Hor Hee¹; Zhi Wei Edwin Ting²; Lawrence Soon-U Lee¹; Jie Xing³; Kelvin Loh Shun Cheng⁴; Zhaoqi Zhan³; ¹Clinical Analysis Centre, Department of Medicine Research Laboratories, National University of Singapore, Singapore, Singapore; ²Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; ³Shimadzu Asia Pacific, Singapore, Singapore; ⁴School of Physical and Mathematical Science, Nanyang Technical University, Singapore, Singapore
- ThP 080 **Multiplexed Quantification of Anti-Tuberculosis (anti-TB) Drugs in Plasma and Tissue via LC-MS/MS Analysis**; Pamela Hummert¹; Mark Marzinke²; ¹Johns Hopkins University, Baltimore, MD; ²Johns Hopkins University, Baltimore, MD



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- ThP 081 **Multiplex Tandem Mass Spectrometry Assays of Six Protein and Glycosaminoglycan Degrading Lysosomal Enzymes in Dried Blood Spots for Newborn Screening;** Frantisek Turecek¹; Yang Liu¹; Fan Yi¹; Ronald Scott¹; Michael H Gelb¹; ¹University of Washington, Seattle, WA
- ThP 082 **New approaches for Enzyme Replacement Therapy of Lysosomal Diseases by Identification and Affinity Quantification of Antibody Epitopes** ; Michael Przybylski¹; Zdenek Kukacka¹; Stefan Maeser¹; Fabio Borri^{1,2}; Lorenzo Altamore²; Julia Hennermann³; Anna Maria Papini²; ¹Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; ²Department of Peptide Chemistry and Biology, University of Florence, Florence, Italy; ³Unimedizin, Villa Metabolica, Universität Mainz, Mainz, Germany
- ThP 083 **Improving Accuracy of Reference Measurements for Serum 25-Hydroxyvitamin D Metabolites by Switching from Solvent- to Serum-Based Calibration** ; Ekaterina Mineva¹; Rosemary Schleicher¹; Shahzad Momin¹; Khin Maw¹; ¹Centers for Disease Control and Prevention, Atlanta, Ga
- ThP 084 **Evaluation of Blood Lysis Procedures prior to Automated Sample Preparation for Immunosuppressant Assay by LC-MS/MS;** Eishi Imoto¹; Mikael Levi¹; Atsuhiko Toyama¹; Daisuke Kawakami²; Jun Watanabe¹; ¹Shimadzu Corporation., MS BU, Kyoto, Japan; ²Shimadzu, Kyoto, Japan
- ThP 085 **Detection and Quantification of Carbohydrate Deficient Transferrin by MALDI-Compatible Protein Chips Prepared by Ambient Ion Soft Landing;** Petra Darebna^{1,2}; Petr Pompach^{1,2,3}; Michal Rosulek^{1,2}; Michael Volny^{1,3}; Petr Novak^{1,2,3}; ¹BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; ²Faculty of Science, Charles University, Prague, Czech Republic; ³Affipro s.r.o., Mratin, Czech Republic
- ThP 086 **Fully Automated Platform for Sensitive Determination of Immunosuppressant Drugs in Whole Blood, Using High Quality Internal Standardization;** Aurore Jaffuel¹; Marc Fernandez¹; Alban Huteau¹; ¹Shimadzu France, Paris, France
- ThP 087 **Evaluation of Interaction of Hop Botanical Dietary Supplements with Drug Metabolism in Women;** Luying Chen¹; Alyssa Tonsing-Carter¹; Richard van Breemen¹; ¹University of Illinois College of Pharmacy, Chicago, IL
- ThP 088 **Single Assay Measurement of Aldosterone-to-Renin Ratio by Online SPE-UHPLC-MS/MS;** Mikael Levi¹; Nicola Gray²; Oneal Joseph³; Ichiro Hirano¹; ¹Shimadzu Corp., MS BU, Kyoto, Japan; ²Shimadzu UK Limited, Milton Keynes, UK; ³Health Services Laboratory, London, UK
- ThP 089 **Quantitative and Rapid Carbapenem Susceptibility Test for Bacteria Based on LDI-TOF MS;** Jong Min Park¹; Joo-Yoon Noh¹; Mira Kim¹; Moon-Ju Kim¹; Jae-Chul Pyun¹; ¹Yonsei University, Seoul, South Korea
- ThP 090 **Fully Automated Platform for Determination of Tricyclic Antidepressant in Serum;** Davide Vecchiotti¹; Claudio Ghilardi²; Katharina Kern³; Stéphane Moreau⁴; Isabel Cabruja²; ¹Shimadzu, Milan, Lombardy; ²Shimadzu Italy, Milan, Italy; ³Recipe Chemicals + Instruments GmbH, Munich, Germany; ⁴Shimadzu Europe GmbH, Duisburg, Germany
- ThP 091 **Comparison of FIA and On-Column LC-MS/MS Method to Measure Simultaneously ABG, ASM, GAA, GALC, GLA and IDUA Activities;** Misa Tanaka¹; Osamu Ohara²; Jun Watanabe¹; Toshikazu Minohata¹; Eishi Imoto¹; Junichi Masuda¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Kazusa DNA Research Institute, Kisarazu, Japan
- ThP 092 **LC-MS-MS Quantitative Analysis of Folic Acid, its Metabolites and Derivatives in Serum for Research Use;** Rory M Doyle¹; Catherine Riley¹; ¹Thermo Fisher Scientific, Somers, NJ
- ThP 093 **Fully Automated Online Sample Preparation AND Quantification of Amiodarone from Whole Blood Using CLAM-LC-MS/MS;** Christian Bunse¹; Lars Kröner²; ¹Shimadzu Deutschland GmbH, Duisburg, Germany; ²Labor Dr. Wisplinghoff, Cologne, Germany
- ThP 094 **Detection of Vitamin D Metabolites Based on Dried Blood Spot Sampling in Combination with LC/MS/MS High-Throughput Analysis;** Konrad Piotr Kowalski^{1,2}; Tomasz Bienkowski^{1,2}; ¹Masdiag Sp. z o.o., Warszawa, Mazowieckie; ²MS Ekspert Sp. z o.o., Gdańsk, Poland
- ThP 095 **Determination of Plasma DHA Using UPLC-MS/MS in APRT Deficient Patients with Ocular Manifestations;** Margret Thorsteinsdóttir^{1,2}; Unnur A. Thorsteinsdóttir¹; ²Hrafnhildur L. Runolfssdóttir^{1,3}; Finnur F. Eiríksson^{1,2}; Vidar O. Edvardsson^{1,3}; Runolfur Palsson^{1,3}; ¹University of Iceland, Reykjavik, Iceland; ²ArcticMass, Reykjavik, Iceland; ³Landspítali – The National University Hospital of Iceland, Reykjavik, Iceland
- ThP 096 **UHPLC-MS/MS quantitative analysis of estrogen metabolites in human serum;** Alan Wong¹; Lingyi Huang¹; Shuai Wang¹; Caitlin Howell¹; Judy L. Bolton¹; Richard B. van Breemen¹; ¹University of Illinois at Chicago, Chicago, IL
- ThP 097 **High-sensitivity, high-throughput quantitation of catecholamines in plasma by Automatable Derivatization and SPE Coupled to LC-MS/MS for Clinical Research;** Atsuhiko Toyama¹; Mikael Levi¹; Ichiro Hirano¹; Jun Watanabe¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 098 **Monitoring Simvastatin Metabolism using LC/MS as a Diagnostic Tool for Celiac Disease Activity;** Jennifer Sealey Voyksner¹; Joseph A Murray²; Jack Syage³; Chaitan Khosla⁴; ¹ImmunogenX, Durham, NC; ²Mayo Clinic, Rochester, MN; ³ImmunogenX, Newport Beach, California; ⁴Stanford University, Stanford, CA
- ThP 099 **Quantitation of Plasma Metanephrine and Normetanephrine by Derivatization Using an Integrated LC-MS/MS Analyzer Equipped with Fully-Automated Sample Preparation Device;** Taku Tsukamoto¹; Daisuke Kawakami¹; Atsuhiko Toyama¹; ¹Shimadzu Corporation, Kyoto, Japan
- ThP 100 **Fast and Sensitive Method for the LCMS Analysis of Vitamin D;** Tim Schlabach¹; Jinhee Kim¹; ¹Novolytic LLC, West Lafayette, IN
- ThP 101 **Improvement of Stability and Reproducibility of Standard Solutions to Guarantee Robust and Reliable Data in LC-MS Analyses Using READYBEADS;** Jordane Biarc¹; Quentin Enjalbert¹; Chloe Bardet¹; Christelle Jaquet¹; Lou Van Poeck¹; Tanguy Fortin¹; ¹ANALQUANT, Villeurbanne, France
- ThP 102 **Quantitative Determination of Free Hormone Fraction via Biocompatible Solid Phase Microextraction (BioSPME);** Sara Smith¹; Candace Price²; Emily Barrey²; Craig Aurand²; Dave Bell²; ¹Millipore Sigma, Bellefonte, PA; ²MilliporeSigma, Bellefonte, PA
- ThP 103 **Simple and Robust LC-MS/MS Method of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood using Luna Omega Polar C18 Column** ; Xianrong (Jenny) Wei¹; Sean Orłowicz¹; ¹Phenomenex, Inc., Torrance, CA

DISEASE BIOMARKERS

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- ThP 105 **Integrated Metabolomics and Metallomics Analysis in Acute Coronary Syndrome Patients;** SAM LI¹; Xuejiao Yin¹; Leonardo Pinto de Carvalho¹; Mark Chan¹; ¹National University of Singapore, Singapore, Singapore
- ThP 106 **Quantitative Proteomics of Murine Exosomes Following Aerosol Exposure to 4,4'-Methylene Diphenyl Diisocyanate;** Brandon F. Law¹; Chen-Chung Lin¹; Paul D. Siegel¹; Justin M. Hettick¹; ¹NIOSH, Morgantown, WV



- ThP 107 **Inhaled 4,4'-Methylene Diphenyldiisocyanate Particulates Haptenate Serum Albumin at Lys535 in Murine Bronchoalveolar Lavage Fluid;** Justin M. Hettick¹; Brandon F. Law¹; Chen-Chung Lin¹; Paul D. Siegel¹; ¹NIOSH, Morgantown, WV
- ThP 108 **A Comprehensive Protein Biomarker Study of Cerebrospinal Fluid from Smith-Lemli-Optiz Patients;** Alfred L. Yergey¹; Stephanie M. Cologna²; Melissa R. Pergande²; Matthew T. Olson³; Peter S. Backlund¹; Christopher A. Wassif¹; Brian C. Searle⁴; Jacqueline A. Picache^{1,5}; Kathryn R. Burkert¹; Vadiraja Bhat⁶; Carol Haney-Ball⁶; Forbes D. Porter¹; ¹National Institutes of Health, Bethesda, MD; ²University of Illinois at Chicago, Chicago, IL; ³Johns Hopkins University, Baltimore, MD; ⁴Proteome Software, Portland, OR; ⁵Vanderbilt University, Nashville, TN; ⁶Agilent Technologies, Wilmington, DE
- ThP 109 **Tegumentray Leishmaniasis Investigated by DESI Imaging and Profile;** Fernanda Negrão¹; Daniele F. de O. Rocha¹; Célio F. F. Angolini¹; Caroline F. Jaeger¹; Daniel R. Abánades¹; Selma Giorgio¹; Marcos N. Eberlin¹; ¹UNICAMP, Campinas, SP
- ThP 110 **Discovering Novel Immunotherapy Targets for Multiple Myeloma with Cell Surface Capture Technology and Parallel Reaction Monitoring Mass Spectrometry;** Nathan J. Schuld¹; Theodore R. Keppel¹; Ensaf M. Hujaili¹; Parameswaran Hari¹; Jeffrey A. Medin¹; Rebekah L. Gundry¹; ¹Medical College of Wisconsin, Milwaukee, WI
- ThP 111 **Novel Biomarkers for Respiratory Diseases Discovered by Secondary Electrospray Ionization – High Resolution Mass Spectrometry;** Nora Nowak¹; Martin T. Gaugg¹; Lukas Bregy¹; Tobias Bruderer¹; Pablo Martinez-Lozano Sinues¹; Alexander Möller²; Malcolm Kohler³; Renato Zenobi⁴; ¹ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland; ²Kinderspital Zürich, Zurich, Switzerland; ³University Hospital Zurich, Zurich, Switzerland; ⁴ETH Zurich, Zurich
- ThP 112 **Localization of Disease Biomarkers in Juvenile Cystic Kidney Using Tissue Mass Spectrometry Imaging;** Cristina I. Silvescu¹; Hanlan Liu¹; Thomas Natoli²; Laurie Smith²; Mandy Cromwell³; Dinesh Bangari⁴; Susan Ryan⁴; Petra Oliva⁵; Lili Guo⁶; Alla Kloss⁶; Thomas O'Shea¹; Walter Korfmacher¹; ¹Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; ²Rare Renal and Bone Disease Research, Sanofi, Framingham, MA; ³Rare Disease Pharmacology, Sanofi, Waltham, MA; ⁴Pathology, Sanofi, Framingham, MA; ⁵Biological Mass Spectrometry, Sanofi, Framingham, MA; ⁶Analytical Research and Development, Sanofi, Waltham, MA
- ThP 113 **Ratiometric Mass Spectrometry Determination of GALE Activity;** Ruth Gordillo¹; Yi Zhu¹; Preethi Csudae¹; Benjamin J. Figard²; Jone Garate³; Duyen Do¹; Philipp E. Scherer¹; ¹Touchstone Diabetes Center, Department of Internal Medicine, Dallas, Texas; ²Shimadzu Scientific Instruments, Columbia, MD; ³Department of Physical Chemistry, University of the Basque Country, Leioa, Afghanistan
- ThP 114 **Targeted Sphingolipid Profiling of Tumor and Plasma Samples in Murine Lung Carcinoma Model Revealing the Mechanism of Doxorubicin;** Ujjaini Dasgupta¹; Nihal Medatwal²; Avinash Bajaj²; Dipanakar Malakar³; Nihal Pillai³; Sandeep Kumar²; ¹Gurgaon, Haryana; ²Regional Center for Biotechnology, Faridabad, India; ³SCIEX, 121, Udyog Vihar, Phase IV., Gurgaon, India
- ThP 115 **Quantitative Analysis of ALS/FTD C9orf72 Protein Isoforms in Cynomolgus Monkey Brain Tissue by Nano-LC and Triple Quadrupole Mass Spectrometer ;** Rong-Fang Gu¹; Alexander McCampbell²; Mia M. Rushe²; Peter Juhasz²; Ru Wei²; ¹Biogen, Cambridge, MA; ²Biogen, Cambridge, MA
- ThP 116 **Identification and functional assay of missing proteins in cancer research;** Yu-Chang Tyan¹; Ming-Hui Yang¹; Po-Chiao Huang¹; ¹Kaohsiung Medical University, Kaohsiung, Taiwan
- ThP 117 **Large-Scale Analysis of Protein Conformational Changes for Biomarker Discovery in Breast Cancer;** Fang Liu¹; Michael C. Fitzgerald¹; ¹Duke University, Durham, NC
- ThP 118 **Proteomic Analysis of Right-Side and Left-Side Colon Cancer Tumors;** Katelyn Ludwig¹; Heinz-Josef Lenz²; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN; ²University of Southern California, Los Angeles, CA
- ThP 119 **Enrichment of Hydrophobic Endogenous Peptides in Urine from Patients with Severe Preeclampsia by Mesoporous Silica Chips;** Hongwu Jing¹; Irina A. Buhimschi²; Guomao Zhao²; Megan Locke²; Sten Heinze²; Jason Sakamoto³; Catalin S. Buhimschi⁴; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Center for Perinatal Research, The Research Institute at Nationwide Children's Hospital, Columbus, OH; ³NanoMedical Systems, Houston, TX; ⁴Department of Obstetrics and Gynecology, The Ohio State University, Columbus, OH
- ThP 120 **Experiment Design and Quality Control for a Large Scale Cancer Proteomics Project: A How-To Guide;** Bin Fang¹; Victoria Izumi¹; Paul A Stewart¹; Robbert JC Slebos¹; Eric A Welsh¹; Ling Cen¹; Yonghong Zhang¹; Zhihua Chen¹; Chia-Ho Cheng¹; Fredrik Pettersson¹; Anders Berglund¹; Guolin Zhang¹; Sean Yoder¹; Katherine Fellows¹; Ann Y. Chen¹; Jamie K Teer¹; Steven Eschrich¹; John Koomen¹; Eric B Haura¹; ¹H. Lee Moffitt Cancer Center, Tampa, FL
- ThP 121 **Affinity Capture MRM Analysis of Molecular Forms of B-type Natriuretic Peptide;** Billy J Molloy¹; James Langridge¹; Leong L Ng²; Thomas Walther^{3,4}; Johannes PC Vissers¹; Donald JL Jones^{2,5}; Toru Suzuki^{2,6}; ¹Waters corporation, Wilmslow, UK; ²Department of Cardiovascular Sciences, University of Leicester, NIHR Leicester Cardiovascular Biomedical Research Unit, Glenfield Hospital, Leicester, UK; ³Department of Pharmacology and Therapeutics, University College Cork, Cork, Ireland; ⁴Institute of Medical Biochemistry and Molecular Biology, University Medicine Greifswald, Greifswald, Germany; ⁵Department of Cancer Studies, RKCSB, University of Leicester, Leicester, UK; ⁶Jichi Medical University, Tochigi, Japan
- ThP 122 **Investigating the Metabolic Links between Insulin Dysregulation, Obesity, and Laminitis in Welsh Ponies via Mass Spectrometry and Statistical Models;** Kevin Murray¹; Sarah Jacob²; Ray Geor³; Elaine Norton¹; Nichol Schultz¹; Molly McCue¹; ¹University of Minnesota, Minneapolis, Minnesota; ²Michigan State University, Lansing, MI; ³Massey University College of Science, Palmerston North, New Zealand
- ThP 123 **Proteomic Analysis of Exosomes Derived Alzheimer's Disease Brain Tissue;** Manveen K Sethi¹; Annina DeLeo²; Tsuneya Ikezu²; Joseph Zaia¹; ¹Center for Biomedical Mass Spectrometry, Department of Biochemistry, Boston University School of Medicine, Boston, MA; ²Department of Pharmacology & Experimental Therapeutics, Boston University School of Medicine, Boston, MA
- ThP 124 **Stratifying Sporadic Amyotrophic Lateral Sclerosis Patients by Metabotype—First Step Towards Developing Personalized Precision Medicine for Effective New Therapies;** Qiuying Chen¹; Davinder Sandhu¹; Benjamin I Schwartz¹; Csaba Konrad¹; Giovanni Manfredi¹; Steven S Gross¹; ¹Weill Cornell Medicine, New York, NY
- ThP 125 **Application of a Comparative Lipidomic Approach to Distinguish Pathogenic Staphylococci;** Naren Gajenthra Kumar¹; Kim Ekroos²; Kimberly Jefferson¹; Dayanjan S Wijesinghe¹; ¹Virginia Commonwealth University, Richmond, VA; ²Lipidomics Consulting Ltd., Irtisvskvägen, Finland



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ThP 126 **A Proteomic Fingerprint of Hormone-Induced Lower Urinary Tract Dysfunction in Mice;** Samuel Thomas¹; Ling Hao²; Dustin Frost²; Paul Marker²; William Ricke^{1,3}; Lingjun Li^{1,2}; ¹*Molecular and Environmental Toxicology Center, University of Wisconsin-Madison, Madison, WI*; ²*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; ³*Department of Urology, University of Wisconsin-Madison, Madison, WI*

ThP 127 **Proteomic Profiling of Plasma, iPSC, 3D Neuron, and Brain Tissue from Alzheimer Patients Using LC-MS/MS;** Mei Chen¹; Han-Kyu Lee¹; Peter Morin¹; John M Wells¹; Eugene B Hanlon¹; Nicole Daniels¹; Lauren Moo¹; Thor Stein^{1,2}; Weiming Xia^{1,3}; ¹*Edith Nourse Rogers Memorial Veterans Hospital, Bedford, MA*; ²*Boston University School of Medicine, Boston, MA*; ³*Boston University School of Medicine, Boston, MA*

ThP 128 **Quantitative Analysis of PZP in Serum: Validation of a Risk Factor for Alzheimer's Disease;** Diana Nijholt¹; Christoph Stingl¹; Peter Koudstaal¹; Peter Sillevs Smitt¹; Arfan M. Ikram¹; Theo M. Luider¹; ¹*Erasmus MC, Rotterdam, Netherlands*

ThP 129 **Mass Spectrometry- based Proteomics of Human Breast Milk for Breast Cancer Biomarker Discovery;** Roshanak Aslebagh¹; Devika Channaveerappa¹; Kathleen F. Arcaro²; Costel C. Darie¹; ¹*Clarkson University, Potsdam, NY*; ²*University of Massachusetts, Amherst, Amherst, MA*

ThP 130 **Predicting Childhood Asthma Using Urine Proteomics;** Tess Kelly¹; Brooke Thompson¹; Paulos Chumala¹; Oluwafemi Oluwale¹; Anna Afanasieva¹; Donna Rennie²; Joshua Lawson¹; George S. Katselis¹; ¹*CCHSA/ Department of Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada*; ²*CCHSA and College of Nursing, University of Saskatchewan, Saskatoon, SK, Canada*

ThP 131 **The Role of Free Fatty Acids in Pulmonary Fibrosis;** Hyun Ju Yoo; *Biomedical Research Center, Asan Institute for Life Sciences, Asan Medical Center, Seoul, South Korea*

DRUG AND METABOLITE ANALYSIS: NOVEL APPROACHES FOR DRIED BIOLOGICAL SAMPLES

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ThP 132 **Elimination of Hematocrit Effect using Volumetric Absorptive Microsampling for the Determination of Ritonavir and Naproxen in Whole Blood by LC-MS/MS;** Nikolay Youhnovski¹; Laurence Mayrand Provencher¹; Eugénie Raphaëlle Bérubé¹; Jeff Plomley¹; Milton Furtado¹; Anahita Keyhani¹; ¹*Altasciences, Laval, QC, Canada, Canada*

ThP 133 **PaperSpray Technology for the Study of Selective High Affinity Ligands (SHALs) and their Metabolites;** Maria C. Prieto Conaway¹; Kerry M Hassell²; Rodney Balhorn³; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Somerset, NJ*; ³*SHAL Technologies, Inc., Livermore, CA*

ThP 134 **Paper Spray Mass Spectrometry for Screening of Antifungal Drugs from Plasma Samples;** Christine Skaggs; *Indianapolis, IN*

ThP 135 **Post-mortem Drug Screening Using Paper Spray MS on a Q-Orbitrap Mass Spectrometer;** Josiah McKenna¹; Rachel Potter¹; Nicholas Manicke¹; ¹*IUPUI, Indianapolis, IN*

ThP 136 **An Integrated Dried Blood Spot (DBS) Collection, Storage and Extraction Device— Towards an Automated Work Flow for Capillary Blood Samples;** Ricardo Neto^{1,2}; Wei Boon Hon^{1,3}; Hans-Jürgen Wirth^{1,3}; Andrew Gooley^{1,3}; Florian Lapierre^{1,4}; Robert Shellie^{1,3}; R. Dario Arrua^{1,2}; Emily F., Hilder^{1,2}; ¹*ARC Training Centre for Portable Analytical Separation Technologies, 7 Argent Place, Ringwood, 3134, Australia*; ²*University of South Australia, Mawson Lakes Campus, Adelaide 5001,*

Australia; ³*Trajan Scientific and Medical, 7 Argent Place, Ringwood, 3134, Australia*; ⁴*University of Tasmania, Sandy Bay, Hobart, 7005, Australia*

ThP 137 **Large Molecule Application of Volumetric Absorptive Microsampling for Single-Rodent PK Profiling of Exenatide Determined by LC-MRM;** Jeff Plomley¹; Daniel Villeneuve¹; Mingluan Chen¹; Kevork Mekhssian¹; Anahita Keyhani¹; Olivier Didur²; William Ruddock²; Luca Genovesi¹; ¹*Algorithme Pharma an Altasciences company, Laval, QC, Canada*; ²*ITR Laboratories, Montreal, QC, Canada*

ThP 138 **Validation of an LC-MS/MS Assay to Monitor Adherence of Subjects on Antiretroviral Therapy Using Dried Blood Spots;** Craig Sykes¹; Amanda Schauer²; Heather MA Prince²; Mackenzie L Cottrell²; Angela DM Kashuba²; ¹*UNC Chapel Hill, Chapel Hill, NC*; ²*UNC Chapel Hill, Chapel Hill, NC*

ThP 139 **LC-MS/MS Combined with Single-Step Extraction Method for the Determination of Nicotine and Cotinine Metabolite in Rat Plasma;** Changyu Quang¹; Kathleen J. McQuate¹; Jennifer L. Simko¹; William C. Nethero¹; Liam B. Moran¹; Elizabeth A. Groeber¹; ¹*Charles River Labs, Ashland, OH*

ThP 140 **Hematocrit Effect: Any Influence in Plasmas Sample Analysis or just a DBS Concern?;** Serge Auger¹; Jean Lacoursiere¹; Pierre Picard¹; ¹*Phytronix Technologies, Quebec, QC, Canada*

ThP 141 **In Tips Micro-Sampling Comparison with Standard Volume Plasma Protein Precipitation with an On-Line Sample Preparation System;** Kimiaka-Chantal Guerard¹; Sylvain Latarte¹; Serge Auger²; Pierre Picard²; ¹*Phytronix Instruments, Boisbriand, QC, Canada*; ²*Phytronix Technologies, Québec, QC, Canada*

ThP 142 **Dried-Blood-Spot Sampling-Device that Solves the Hematocrit-Problem, is Patient Friendly, has Timestamp Functionality, and is Amenable to Complex & Automated Processing;** Lars Liepold; *AmpleSample, Minneapolis, MN*

ThP 143 **Detection of Growth Promoting Agents in Equine Dried Blood Spots Using Liquid Chromatography - Tandem Mass Spectrometry;** Benjamin C Moeller¹; Zicheng Yang²; Amel J Clifford¹; Scott D Stanley¹; ¹*University of California, Davis, School of Veterinary Medicine, KL Maddy Equine Analytical Chemistry Laboratory, Davis, CA*; ²*Bruker Daltonics, Fremont, CA*

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ThP 144 **Comparison of Perfluorinated Compounds in Drinking Water between Triple Quadrupole MS/MS and High Resolution Mass Spectrometry - Knowns and Unknowns;** Ed George¹; Ali Haghani²; Andy Eaton²; ¹*ThermoFisher Scientific, San Jose, CA*; ²*Eurofins Eaton Analytical, Monrovia, California*

ThP 145 **What Role Does Hydrogen Have in the Embrittlement of Nuclear Reactor Components? ;** Richard Cox¹; Grant Bickel²; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Canadian Nuclear Laboratory, Chalk River, Ontario*

ThP 146 **Disinfection By-Products of Aquatic Chlorination and Bromination of UV Filter Avobenzene;** Albert T. Lebedev¹; Anastasia Chugunova¹; Olga Polyakova¹; Viatcheslav Artaev²; Polonca Trebse³; ¹*Moscow State University, Moscow, Russia*; ²*LECO Corporation, St. Joseph, MI*; ³*University of Ljubljana, Ljubljana, Slovenia*

ThP 147 **Low Level Quantification of NDMA and Non-Targeted Contaminants Screening in Drinking Water Using GC-Orbitrap-Mass Spectrometry;** Dan Quinn; *Thermo Fisher Scientific, Chardon, OH*

ThP 148 **Expanding Horizons in Real Time Analysis: Dual Polarity SIFT-MS;** Murray J Mcewan¹; Thomas I McKellar²; Vaughan S Langford²; David Hera²; Daniel B Milligan²;



- ¹University of Canterbury, Christchurch, Canterbury; ²Syft Technologies Ltd, Christchurch, New Zealand
- ThP 149 **Development of a Complete Method Validation for the use of Solid Phase Extraction with EPA 625.1;** Philip Bassignani¹; Rudolf Addink¹; ¹Toxic Report, Watertown, MA
- ThP 150 **Screening for Water Contaminants by All-Ion Fragmentation in Rhine River Samples;** Sylvain Merel¹; Gina Di Napoli-Davis¹; Christian Zwiener¹; ¹Universität Tübingen, Tübingen, Germany
- ThP 151 **A Sensitive and Automation Approach Using large Volume Injection System Couple with LC-MS/MS to Analyze Perfluorinated Compounds in Environmental Samples;** Wen-Yen Lee¹; Dai-Yong Huang²; Yanan Yang³; Shan-An Chan¹; ¹Agilent Technologies Inc., Taipei, Taiwan; ²Agilent Technologies Ltd. Hong Kong, Hong Kong, Hong Kong; ³Agilent Technologies Inc., Santa Clara, CA
- ThP 152 **Screening for Dioxin-Like Compounds in Sediment Using Modified QuEChERS and a GC-TOF Mass Spectrometer with Atmospheric Pressure Chemical Ionization ;** Liad Haimovici¹; Karl Jobst¹; Eric Reiner¹; Karen MacPherson¹; Jack Cochran²; ¹Ontario Ministry of the Environment and Climate Change, Toronto, ON, Canada; ²VUV Analytics, Inc., Austin, TX
- ThP 153 **Analysis of Dioxins, Furans and Polychlorinated Biphenyls in Sediments and Fish Using the Novel 7250 High-Resolution GC/Q-TOF;** Peter Haglund¹; Sofia Nieto²; Nathan Eno²; ¹Umeå University, Umeå, Sweden; ²Agilent Technologies, Inc., Santa Clara, CA
- ThP 154 **Extraction and Analysis of Poly Brominated Diphenyl Ether in Aqueous Samples Using EPA 1614;** Rashid Juma¹; Rudolf Addink¹; ¹Toxic Report, Watertown, MA
- ThP 155 **Identification of Halogenated Disinfection Byproducts of Nonylphenol in Chlorinated Wastewater Effluent Using a Novel High Resolution GC/Q-TOF;** Christiane Hoppe-Jones¹; Sofia Nieto²; Nathan Eno²; Craig Marvin³; Shane Snyder¹; ¹University of Arizona, Tucson, AZ; ²Agilent Technologies, Inc., Santa Clara, CA; ³Agilent Technologies, Inc., Wilmington, DE
- ThP 156 **Application of a Non-Targeted Screening Workflow to Identify Toxic Contaminants in Waste Water Effluent;** Bernadette Vogler¹; Christian Götz²; Bernd Kobler³; Heinz Singer¹; ¹EAWAG, Dübendorf, ZH; ²Envilab AG, Zofingen, Switzerland; ³GVRZ, Cham, Switzerland
- ThP 157 **Analysis of Combustion Byproducts on Firefighter Protection Equipment Using a Novel High Resolution GC/Q-TOF;** Christiane Hoppe-Jones¹; Sofia Nieto²; Nathan Eno²; Shane Snyder¹; ¹University of Arizona, Tucson, AZ; ²Agilent Technologies, Inc., Santa Clara, CA
- ThP 158 **Detection of Novel Perfluorinated Ether Sulfonates in Wildlife in South Carolina and Florida;** Jackie Bangma¹; Jessica L Reiner²; Russell H Lowers³; John A. Bowden²; ¹Charleston, SC; ²National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; ³Integrated Mission Support Services, Titusville, FL
- ThP 159 **Analysis of Compounds Derived from Aquatic Plastic Pollution by GC-TOFMS;** Kathryn M Renyer¹; John J Kelly¹; Timothy J Hoellien¹; Daryl Giblin²; M. Paul Chiarelli¹; Michael L. Gross^{2,3}; ¹Loyola University, Chicago, IL; ²Washington University, St Louis, MO; ³Washington University School of Medicine, St Louis, MO
- ThP 160 **Evaluation of a Novel Combination Sampler/ Reagent with Liquid Chromatography Coupled to Tandem Mass Spectrometry Detection to Measure 4,4'-Methylenediphenyldiisocyanate Atmospheres;** Sebastien Gagne¹; Silvia Puscasu¹; Simon Aubin¹; Philippe Sarazin¹; Mark Spence²; ¹IRSS, Montreal, Qc; ²III, Manchester, UK
- ThP 161 **Mass Fragment and Neutral Loss Database for Non-Target Environmental Analysis by Liquid Chromatography/High Resolution Mass Spectrometry;** Shigeru Suzuki¹; Mari Takazawa¹; Atsuko Hasegawa²; Michiko Uebori¹; Yasuko Yoshida³; Masahiko Takino⁴; Kaori Okubo⁵; Miho Shinomiya⁶; ¹Chubu University, Kasugai, Aichi; ²Kanagawa Environmental Research Center, Hiratsuka, Japan; ³Sumica Chemical Analysis Service Ltd., Tokyo, Japan; ⁴Agilent Technologies Japan Ltd., Hachioji, Japan; ⁵Saga Pharmaceutical Sanitation Center, Saga, Japan; ⁶Saitama Prefectural University, Kasukabe, Japan
- ThP 162 **Two-Dimensional Liquid Chromatography Coupled with High-Resolution Mass Spectrometry: Application for Analysis of Complex Surfactant Mixtures in Aquatic Environments;** Sarah Choyke¹; Bernadette Vogler²; Gordon Getzinger¹; P. Lee Ferguson¹; ¹Duke University, Durham, NC; ²EAWAG, Dübendorf, ZH
- ThP 163 **Analysis of Arsenic and Thioarsenic Species in Sulfidic Waters using Liquid Chromatography Mass Spectrometry;** Akeena Harper¹; Denzel Bolden¹; JIANYE ZHANG¹; ¹Voorhees College, Denmark, SC
- ThP 164 **Non-Targeted Screening of More than 20 Ethoxylated Homologs and their Transformation Products in Water Samples Using High Resolution-Mass Spectrometry;** Maryam Khaksari^{1,2}; Lynn R Mazzoleni^{1,2}; ¹Chemical Advanced Resolution Methods, Michigan Technological University, Houghton, Michigan; ²Department of Chemistry, Michigan Technological University, Houghton, MI
- ThP 165 **Validation of a Thermal Desorption GC/MS Method for the Analysis of Chemical Warfare Agents (CWAs) ;** Thomas Rusek¹; Jonathan Oyler²; ¹Battelle/ MRICD, Aberdeen, MD; ²APG, Edgewood, MD
- ThP 166 **Surpassing Detection Limits for 200 Organic Compounds in Water Using EPA Method 525.2 via GC/ MS;** Lorne Fell¹; Todd Richards²; Joe Binkley²; ¹LECO, St. Joseph, Michigan; ²LECO Corporation, Saint Joseph, MI
- ThP 167 **The Analysis of Environmental Samples Using High Resolution Mass Spectrometry to Identify Novel PFAS Compounds;** Paul C. Winkler¹; Simon Roberts¹; Craig Butt¹; Christopher Borton¹; ¹SCIEX, Framingham, MA
- ThP 168 **Gas Chromatography Mass Spectrometry Analysis of Volatile Arsenic-Sulfur Species in Environments of High Levels of Sulfide;** Shelia J Jamison¹; Yaoling Long²; Jianye Zhang¹; ¹Voorhees College, Denmark, SC; ²South Carolina State University, Orangeburg, SC
- ThP 169 **High Resolution Mass Spectrometry Discovery of N-Halogenated-Peptides in Drinking Water;** Ping Jiang¹; Guang Huang¹; Lindsay Jmaiff Blackstook¹; Xing-Fang Li²; ¹University of Alberta, Edmonton, Alberta; ²University of Alberta, Edmonton, AB, Canada
- ThP 170 **Qualitative Analysis of Halogenated Organic Compounds Unintentionally Generated in Municipal Waste Water Treatment Plants;** Mari Takazawa¹; Shigeru Suzuki¹; Takeshi Nakano²; Shinji Tsunoi²; Miho Shinomiya³; ¹Chubu University, Kasugai, Japan; ²Osaka University, Research Center for Environmental Preservation, Suita, Japan; ³Saitama Prefectural University, Kasukabe, Japan
- ThP 171 **Structural Elucidation and Differentiation of Azo Disperse Dyes Containing Different Substituents at the Benzene Core;** Nadia Sultana¹; Nelson R. Vinuesa¹; ¹Department of Textile Engineering, Chemistry and Science, NC State University, Raleigh, NC
- ThP 172 **Development of a Cigarette Smoke Constituent Analysis Method in Combined Particulate and Gas Phase Smoke in Nose-Only Exposure Chamber;** Yongquan Lai¹; Edward Yates¹; Larry Mallis¹; Hammad Irshad¹; Philip Kuehl¹; Tyler Sniegowski¹; Jacob McDonald¹; ¹Lovelace Biomedical, Albuquerque, NM
- ThP 173 **Molecular-level Insights into the Increased Toxicity of Crude Oil Environmental Transformation Products;** Phoebe Zito¹; Huan Chen¹; Amy M McKenna¹; David C Podgorski^{1,2}; Steven M. Rowland^{1,3}; Jie Lu³; Yuri E Corilo^{1,3}; Ryan P. Rodgers¹; ¹National High Magnetic Field Laboratory,



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- ThP 174 **Determination of Per/Polyfluoroalkyl Substances (PFAS) in Water Using HPLC/MS/MS;** Tarun Anumol¹; Theresa Sosienski²; Craig Marvin¹; Dan-Hui Dorothy Yang²; Patrick Jeanville²; ¹Agilent Technologies, Inc., Wilmington, DE; ²Agilent Technologies, Inc., Santa Clara, CA
- ThP 175 **Determination Nitrosamines in Drinking Water by GC-Triple Quadrupole Mass Spectrometry;** Louis Maljers¹; Steve Fannin²; ¹Bruker Daltonics, andover, ma; ²Bruker Daltonics, Billerica, MA

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- ThP 176 **Probing Non-Covalent Binding Interactions between Anionic Phosphate and Cationic Guanidinium using UV-Vis Photodissociation in Combination with Molecular Dynamic Simulations;** Huong (Ivy) Thi Huynh Nguyen¹; Frantisek Turecek²; ¹University of Washington, Department of Chemistry Seattle, WA; ²University of Washington, Department of Chemistry, Seattle, WA
- ThP 177 **Preferential Cleavage at Lysine Residues Upon Activation of [M-H-NH3]⁺ derived from Ion/Ion Reactions with the Gold Dichloride Reagent Anion.;** David J Foreman¹; Stella K Betancourt¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, Indiana
- ThP 178 **Distinguishing Hexosamines and N-Acetylated Hexosamines Using a Simple Ion/Molecule Reaction;** Aditya M. Anerao¹; Matthew T. Campbell¹; Gary L. Glish¹; ¹University of North Carolina, Chapel Hill, NC
- ThP 179 **Identification of Phospho- and Sulfopeptides via Charge Inversion Ion/Ion Reactions and Dipolar DC Collisional Activation;** Mack Shih¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, Indiana
- ThP 180 **Reactions of Sulfur-Containing Organic Anions with Hydrogen, Nitrogen, and Oxygen Atoms;** Yake Li^{1,2,3}; Zhechen Wang¹; Shenggui He²; Veronica M. Bierbaum¹; ¹Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO; ²Institute of Chemistry, Chinese Academy of Sciences, Beijing, China; ³University of Chinese Academy of Sciences, Beijing, China
- ThP 181 **The Dissociation and Ion Molecule Reaction Pathways of Gas-Phase Complexes Composed of Alkaline Earth Metals Coordinated by Alcohol Ligands;** Sarah Sheffield¹; Susan Kline¹; Jordan Pestok¹; Michael Van Stipdonk¹; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA
- ThP 182 **A Gas-Phase Study of the Nucleophilic Halogenation of Aromatic Heterocycles;** Leah Donham¹; Scott Gronert¹; ¹Virginia Commonwealth University, Richmond, VA
- ThP 183 **Electrospray-Based Photo-Catalytic Screening Method for Studying Electronic Effects on Oxidative Dehydrogenation of N-heterocycle Compounds;** Savithra Jayaraj¹; Abraham K. Badu-Tawiah²; ¹The Ohio State University, Columbus, OH; ²The Ohio State University, Columbus, OH
- ThP 184 **Exploring Gas Phase Behavior of Small Cationized Non-Covalent Complexes between Hexose-Phosphate and Basic Compounds Using H/D Exchanges;** Ekaterina Dary^{1,2,3}; Yves Gimbert⁴; Sandra Alves⁵; Alain Perret^{1,2,3}; Jean-Claude Tabet⁶; ¹Commissariat à l'Energie Atomique et aux Energies Alternatives, Direction de la Recherche Fondamentale, Institut de Génomique, Evry, France; ²Université d'Evry Val d'Essonne, Evry, France; ³Centre National de la Recherche Scientifique, UMR8030, Génomique métabolique, Evry, France; ⁴Université Grenoble Alpes (DCM), CNRS-UJF 5250, BP 38041,

Grenoble, France; ⁵Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire, Paris, France; ⁶Commissariat à l'Energie Atomique et aux Energies Alternatives, iBiTec-S, SPI, LEMM, Gif Sur Yvette, France

- ThP 185 **Going Where Few Dare To: Exploring the Intrinsic Reactions of Uranyl-Oxo and -Oxo Hydride Anions with H₂O and O;** Michael J. Van Stipdonk¹; Evan Perez²; Cassandra Hanley¹; Irena Tatosian¹; Amanda Bubas¹; ¹Duquesne University, Pittsburgh, PA; ²Yale University, New Haven, CT
- ThP 186 **Flame Atmospheric Pressure Chemical Ionization Coupled with Negative Electrospray Ionization Mass Spectrometry for Ion Molecule Reactions;** Sy-Chyi Cheng¹; Suhail Muzaffar Bhat¹; Jentaie Shiea¹; ¹National Sun Yat-Sen University, Kaohsiung, Taiwan
- ThP 187 **Manipulation of conformation via charge and temperature. An ion mobility mass spectrometry investigation;** Jacquelyn R Jhingree¹; Jakub Ujma²; Perdita E Barran¹; ¹University of Manchester, Manchester, UK; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- ThP 188 **A FT-3D Ion Trap with In-Trap Electron Ionization and Pulsed Gas Inlet: Transient Pressure Profile and Space Charge Induced Effects;** Yessica Brachthäuser¹; David Mueller¹; Hendrik Kersten¹; Klaus J. Brockmann¹; Valerie Derpmann²; Michel Aliman²; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW; ²Zeiss SMT GmbH, Oberkochen, Germany
- ThP 189 **Ion Dynamics Simulation: Space Charge Effects in a Fourier Transform 3D-Ion Trap (FT-ion trap);** Walter Wissdorf¹; Christine Polaczek¹; Yessica Brachthäuser¹; Hendrik Kersten¹; Albrecht Brockhaus¹; Michel Aliman²; Valerie Derpmann²; Alexander Laue²; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW; ²Zeiss SMT GmbH, Oberkochen, Germany
- ThP 190 **Systematic Studies of the Impact of Chemical Modifiers on the Ion Population Observed with Nano Electrospray Ionization (nESI) Mass Spectrometry;** Marco Thinius¹; Christine Polaczek¹; Clara Markert¹; Duygu Erdogdu¹; Hendrik Kersten¹; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW
- ThP 191 **Fast Space Charge Simulations: Simulation of Ion – Ion and Background Gas Interaction in a Linear Quadrupole;** Walter Wissdorf¹; Hendrik Kersten¹; Thorsten Benter¹; Tom Covey²; Jim Hager²; Bradley B Schneider²; ¹Bergische Universität Wuppertal, Wuppertal, NRW; ²SCIEX, Concord, ON, Canada
- ThP 192 **Effects of Chemical Dynamics and Clustering Reactions of Chemical Modifiers with Analyte Ions in Differential Mobility Spectrometry (DMS);** Florian Stappert¹; Marco Thinius¹; Hendrik Kersten¹; Walter Wissdorf¹; Tom Covey²; Bradley B Schneider²; Jim Hager²; Thorsten Benter¹; ¹Bergische Universität Wuppertal, Wuppertal, NRW; ²SCIEX, Concord, ON, Canada
- ThP 193 **Characterization of Unusual CO₂ and N₂ Adducts to Gas-phase Copper Ion using Isotope Labeling and High-accuracy Mass Measurements;** Luke Metzler¹; Stephen Koehler¹; Arpad Somogyi²; Michael J. Van Stipdonk¹; ¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; ²Mass Spectrometry and Proteomics Facility, Campus Chemical Instrument Center, Columbus, OH
- ThP 194 **Reactivity of Amino Acid Anions with Atomic Species in the Interstellar Medium;** Zhechen Wang¹; Veronica M. Bierbaum¹; Yake Li¹; ¹University of Colorado at Boulder, Boulder, CO
- ThP 195 **Creation and Intrinsic Reactions of Gas-phase Group II Cation-carbanion Complexes;** Stephen Koehler¹; Cassandra Hanley¹; Nevo Polonsky^{1,2}; Jordan Pestok¹;



- Michael J. Van Stipdonk¹; ¹Duquesne University, Pittsburgh, PA; ²Bates College, Lewiston, ME
- ThP 196 **Gas-phase Rearrangement Reaction of Schiff-Base-Modified Peptide Ions**; Nan Wang¹; Alice L Pilo²; Jiexun Bu¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN; ²Merck & Co., Inc, Rahway, NJ
- ThP 197 **Oxygen Peribridged Quinolinium Biradicals: Gas-Phase Reactivity Study by Using a Linear Quadrupole Ion Trap (LQIT) Mass Spectrometer**; Raghavendhar R Kotha¹; Ravikiran Yerabolu¹; John J Nash¹; Hilkka I Kenttamaa¹; ¹Purdue University, West Lafayette, Indiana
- ThP 198 **Identification of Glucuronidation Sites in Protonated Drug Metabolites by Using Ion-Molecule Reactions and Energy-Resolved Mass Spectrometry**; Edouard Niyonsaba¹; Xin Ma¹; Zaikuan Yu¹; John Kong¹; Hilkka Kenttamaa¹; ¹Purdue University, West Lafayette, IN
- ThP 199 **5-Dehydroquinoline Radical Cation: a New Reactive σ,σ -Biradical Formed via Isomerization from 5-Iodo-8-Dehydroquinolinium Cation**; Xin Ma¹; Chunfen Jin¹; John J. Nash¹; Hilkka I. Kenttamaa¹; ¹Purdue University-Department of Chemistry, West Lafayette, IN
- ThP 200 **Gas-Phase Synthesis and Reactivity of Diphenylphosphonium Cations**; Xinchi Yin¹; Yuanjiang Pan¹; ¹Department of Chemistry, Zhejiang University, Hangzhou, China
- ThP 201 **The tautomerism of Phosphonium Cations in the Gas Phase**; Xinchi Yin¹; Shanshan Shen¹; Yuanjiang Pan¹; ¹Department of Chemistry, Zhejiang University, Hangzhou, China
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- ThP 202 **Hydrogen/Deuterium Exchange Mass Spectrometry: A Sensitive Biophysical Tool to Study Protein-Protein and Protein-Ligand Interactions**; Alfonso Espada¹; Howard Broughton¹; Jeffrey A. Dodge²; Spencer Jones²; Isabel Gonzalez²; Michael Grogan²; Alsina-Fernandez Jorge²; John Lee²; Michael J Chalmers²; ¹Lilly S.A., Alcobendas, Madrid; ²Eli Lilly and Company, Indianapolis, IN
- ThP 203 **Tracking Conformational Dynamics and Ligand Binding in Membrane Proteins Using HDX-MS**; Martin Lorenz Eisinger¹; Layin Nie^{1,2}; Aline Ricarda Doerrbaum^{1,3}; Hartmut Michel¹; Etana Padan⁴; Julian Langer^{1,3}; ¹MPI for Biophysics, Frankfurt am Main, Hessen; ²University of Oxford, Oxford, UK; ³MPI for Brain Research, Frankfurt am Main, Germany; ⁴Hebrew University, Jerusalem, Israel
- ThP 204 **Sequential Conformational Changes in Influenza Hemagglutinin during Fusion Activation**; Mark Benhaim; University of Washington, Seattle, WA
- ThP 205 **Investigation of Interactions between Beta-Lactamases and Beta-Lactamase Inhibitory Protein (BLIP) Using Hydrogen/Deuterium Exchange Mass Spectrometry (HDX-MS)**; Liwen Huang¹; Pui-kin So¹; Yun-chung Leung¹; Zhong-ping Yao¹; ¹The Hong Kong Polytechnic University, Hong Kong, China
- ThP 206 **HDX MS of the Largest Soluble Human Glycoprotein, Von Willebrand Factor**; Roxana E. Iacob¹; Klaus Bonazza²; Timothy A. Springer³; John R. Engen⁴; ¹Northeastern University, Boston, MA; ²Children's Hospital Boston and Harvard Medical School, Boston, MA; ³Children's Hospital Boston and Harvard Medical School, Boston, MA; ⁴Northeastern University, Boston, MA
- ThP 207 **Use of Differential Hydrogen/Deuterium Exchange Mass Spectrometry to Support Ligand Binding Mode Predictions within the Vitamin D Receptor**; Ryan Stites¹; Scott Novick²; Bruce D Pascal²; Quanrong Shen¹; Michael J Chalmers¹; Patrick R Griffin²; Jeffrey A Dodge¹; ¹Eli Lilly and Company, Indianapolis, IN; ²The Scripps Research Institute, Jupiter, FL
- ThP 208 **Hydrogen Deuterium Exchange Mass Spectrometry of ROR γ t Modulators Show Conformational Changes and Allosteric Binding Site**; Rebecca Rae¹; Yafeng Xue²; Anna Aagaard²; Frank Narjes³; ¹Department of Medicinal Chemistry, Respiratory, Inflammation & Autoimmunity, Innovative Medicines and Early Development Biotech Unit, AstraZeneca, Gothenburg, Sweden; ²Discovery Sciences, AstraZeneca, Gothenburg, Sweden; ³Department of Medicinal Chemistry, Respiratory, Inflammation & Autoimmunity, Innovative Medicines and Early Development Biotech Unit, Gothenburg, Sweden
- ThP 209 **Using Hydrogen/Deuterium Exchange-Mass Spectrometry to Probe Changes in Enzyme Dynamics during Catalysis**; Courtney S Fast¹; Siavash Vahidi¹; Lars Konermann¹; ¹University of Western Ontario, London, ON, Canada
- ThP 210 **Conformational Changes in Active/Inactive States of PP2C α Characterized by Hydrogen-Deuterium Exchange Mass Spectrometry**; Kyle W Anderson^{1,2}; Sharlyn J Mazur³; Subrata Debnath³; Elyssia S Gallagher^{1,2}; Stewart R Durell³; Ettore Appella³; Jeffrey W Hudgens^{1,2}; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²IBBR, Rockville, MD; ³National Cancer Institute, Bethesda, MD
- ThP 211 **Development of a Hydrogen Exchange-Mass Spectrometry Method to Predict Aggregation Propensity of Protein Therapeutics**; Juan P Rincon¹; Gulsum Meric²; Cesar Calero-Rubio²; Christopher O'Brien²; Anne Robinson³; Christopher J Roberts²; David D Weis¹; ¹University of Kansas, Lawrence, Kansas; ²University of Delaware, Newark, Delaware; ³Tulane University, New Orleans, Louisiana
- ThP 212 **HDX-MS Reveals a Common Binding Surface for Endogenous Peptide- and Protein Ligands to the Sortilin Receptor**; Esben Trabjerg^{1,2}; Fredrik Kartberg²; Søren Christensen²; Kasper D Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Department of Biologics, H. Lundbeck A/S, Valby, Denmark
- ThP 213 **Pulsed HDX Illuminates the Aggregation Kinetics of Alpha Synuclein, the Causative Agent for Parkinson's Disease**; Eva T. Illes-Toth¹; Don L. Rempel¹; Michael L. Gross¹; ¹Washington University in St Louis, St. Louis, MO
- ThP 214 **Discovery and Structural Analysis of Selective Modulators for Retinoic-Acid Receptor-Related Orphan Receptor ROR β** ; Venkat Dharmarajan¹; Chrsitelle Doebelin¹; Ted Kamenecka¹; Ruben Garcia-Ordonez¹; Patrick R Griffin¹; ¹The Scripps Research Institute, Jupiter, FL
- ThP 215 **Hydrogen Deuterium Exchange of Native Ubiquitin Probed by hv-ECD with Complete Sequence Coverage**; Yury V. Vasil'ev¹; Nathan I. Lopez¹; Valery G. Voinov²; Joseph S. Beckman¹; ¹Linus Pauling Institute, Oregon State University, Corvallis, OR; ²e-MSion, Corvallis, OR
- ThP 216 **Mapping Substrate Binding Sites of Low Affinity Ligands to a Glycosyltransferase Using HDXMS**; Deepa Balasubramaniam¹; Thierry Fischmann¹; Todd Mayhood¹; Michael Kavana²; George Addona²; Maria Webb¹; Payal Sheth¹; David McLaren¹; ¹Merck, Kenilworth, NJ; ²Merck & Co., Inc., Boston, MA
- ThP 217 **Effects of N and C Terminal Truncations on Heme Oxygenase 2 Examined via Hydrogen Deuterium Exchange Mass Spectrometry**; Brent A. Kochert¹; Angela S. Fleischacker²; Stephen W. Ragsdale²; John R. Engen¹; ¹Northeastern University, Boston, MA; ²University of Michigan, Ann Arbor, Michigan
- ThP 218 **HDX-MS and Molecular Dynamics Simulations Provide Complementary Insights Into The Mechanisms of Allosteric Protein Regulation**; Yiming Xiao¹; Gary S Shaw²; Lars Konermann²; ¹University of Western Ontario,



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- London, ON, Canada; ²University of Western Ontario, London, ON, Canada
- ThP 219 **Dissection of Key Conformational Changes in the Regulatory Domains of BTK upon Lipid Interaction: is the Full-Length Kinase Necessary?**; Charles Mundorff¹; Thomas E. Wales¹; Raji E. Joseph²; Amy H. Andreotti²; John R. Engen¹; ¹Northeastern University, Boston, MA; ²Iowa State University, Ames, IA
- ThP 220 **Characterizing the Binding Interface between Human Insulin-like Growth Factor and its Binding Protein by Hydrogen/Deuterium Exchange Mass Spectrometry**; Paul A. Salinas¹; Hanwei Zhao¹; Justin M. Prien¹; Bernice Yeung¹; ¹Shire HGT, Lexington, MA
- ThP 221 **HDX-MS and Quantitative Crosslinking-MS (XL-MS) Reveals NR AF2 Dynamics Controlling Receptor Activity and Target Gene Promoter Specificity**; Jie Zheng¹; Bruce D. Pascal¹; Ruben Garcia-Ordonez¹; Scott Novick¹; Mira Chang¹; Patrick R Griffin¹; ¹The Scripps Research Institute, Jupiter, FL
- ThP 222 **Implementation of HDX-MS and SCA to Elucidate the Role of Allosteric Coupling during Electron Transport in Transhydrogenase Complexes**; Luke Berry¹; Saroj Poudel¹; Monika Tokmina-Lukaszewska¹; Dan Coleman¹; Gerrit J. Schut²; Michael W.W. Adams²; John Peters³; Eric Boyd¹; Brian Bothner¹; ¹Montana State University, Bozeman, MT; ²University of Georgia, Athens, GA; ³Washington State University, Pullman, WA
- ThP 223 **Allosteric Conformational Change of KEAP1 upon Nrf2 Binding Based on Hydrogen/Deuterium Exchange Monitored by 21 T FT-ICR Mass Spectrometry**; Peilu Liu^{1,2}; Mengqi Zhong³; Adrian Whitty³; Alan G. Marshall^{1,2}; ¹Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; ²National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ³Department of Chemistry, Boston University, Boston, MA
- ThP 224 **Application of Hydrogen-Deuterium Exchange Mass Spectrometry to Interrogate the Dynamic Conformational Regulation of BCL-2 Family Proteins**; Susan Lee¹; Lauren A Barclay¹; Thomas E Wales²; Franziska Wachter¹; Gregory H Bird¹; John R Engen²; Loren D Walensky¹; ¹Dana Farber Cancer Institute, Boston, MA; ²Northeastern University, Boston, MA
- ThP 225 **Probing Mutations in the Tec-Family Tyrosine Kinase BTK Using NMR, HXMS, and a Combined Domain Building Block Approach**; Thomas E. Wales¹; Raji E. Joseph²; Amy H. Andreotti²; John R. Engen³; ¹Northeastern University, Boston, MA; ²Iowa State University, Ames, IA; ³Northeastern University, Boston, MA
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- ThP 258 **Bioimaging via LA-ICP-MS - a Powerful Analytical Tool for the Investigation of the Anti-Cancer Drug Cisplatin;** Oliver Bolle Bauer¹; Christina Köppen¹; Giuliano Ciarimboli²; Hans-Joachim Schurek²; Michael Sperling¹; Uwe Karst¹; ¹Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany; ²University Hospital of Münster, Department of Experimental Nephrology, Münster, Germany
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- ThP 260 **Infrared Laser Ablation Microsampling and Data Independent Acquisition Mass Spectrometry for Tissue Proteomics;** Kelin Wang¹; Fabrizio Donnarumma¹; Carson W Szot¹; Michael E. Pettit²; Touradj Solouki²; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA; ²Baylor University, Waco, Texas
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- ThP 263 **Implementation of a Novel Scanning Quadrupole Data Independent Acquisition Method for DESI imaging;** Mark Towers¹; Emrys Jones¹; Philippa Hart¹; Michael Batey¹; Emmanuelle Claude¹; James Langridge¹; ¹Waters Corporation, Wilmslow, UK
- ThP 264 **An Investigation into MALDI Imaging Sample Preparation Compared to DESI Imaging for Multimodal MSI in Pre-clinical Breast Cancer Research;** Mark W Towers¹; Philippa J Hart¹; Jonathan Sleeman²; Kirill A Veselkov³; Emmanuelle Claude¹; ¹Waters Corp., Wilmslow, UK; ²Center for Biomedicine and Medical Technology



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- ThP 267 **Three Steps to Enhanced Ganglioside Species Detection by MALDI Imaging Mass Spectrometry**; Ethan Yang¹; Martin Dufresne¹; Pierre Chaurand¹; ¹Department of Chemistry, Université de Montréal, Montréal, QC, Canada
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- ThP 273 **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
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- ThP 275 **Mass Spectrometry Imaging Reveals the Sub-Organ Distribution of Carbon Nanomaterials**; Suming Chen¹; Caiqiao Xiong²; Huihui Liu²; Qiongqiong Wan³; Jian Hou²; Qing He²; Abraham K. Badu-Tawiah³; Zongxiu Nie²; ¹School of Medicine, Johns Hopkins University, Baltimore, MD; ²Institute of Chemistry, Chinese Academy of Sciences, Haidian, China; ³The Ohio State University, Columbus, OH
- ThP 276 **Optimized MALDI IMS Protocol for Breast and Ovarian Cancer Tissue Obtained by a Two-Center Method Development And Reproducibility Study**; Delf Lachmund¹; Rita Casadonte²; Janina Oetjen¹; Lena Hauberg-Lotte¹; Tobias Boskamp^{1,3}; Dennis Trede³; Joerg Kriegsmann^{2,4}; Peter Maass^{1,3}; ¹University of Bremen, Bremen, Germany; ²ProteoPath GmbH, Trier, Germany; ³SCiLS GmbH, Bremen, Bremen; ⁴Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany
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- ThP 278 **In situ Labeling for the Absolute Quantitation of Crustacean Neuropeptides with Mass Spectrometric Imaging**; Amanda Buchberger¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 279 **Method Development for Quantitative Investigation of Terbinafine Hydrochloride in a 3D Skin Model by MALDI-MSI**; Cristina Russo¹; Stephan Rumbelow²; Steve Mellor³; Catherine Duckett⁴; Neil Bricklebank⁴; Malcolm Clench⁴; ¹Sheffield Hallam University, Sheffield; ²Croda Inc. Griffin Innovation Center, New Castle, DE 19720; ³Croda Europe Ltd., Snaith Goole, UK; ⁴Sheffield Hallam University, Sheffield, UK
- ThP 280 **Material Transport in LMD-LVC/ESI-MS and its Impact on Collection Efficiency and Quantitative MS Imaging**; John F. Cahill¹; Vilmos Kertesz¹; Gary J. Van Berkel¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 281 **From Imaging Peaks to Molecules: Parallelised MALDI-FTMS-MSI and MS/MS Enables Broad Structure Elucidation and Differential Imaging of Lipid Isomers**; Shane R. Ellis¹; Martin R. L. Paine¹; Christer S. Ejlsing²; Berwyck Poad³; Stephen J. Blanksby³; Ron M. A. Heeren¹; ¹M4I Institute - Maastricht University, Maastricht, Netherlands; ²Department of Biochemistry and Molecular Biology, VILLUM Center for Bioanalytical Sciences University of Southern Denmark, Odense, Denmark; ³Queensland University of Technology, Brisbane, Australia
- ThP 282 **Histology Directed Liquid Surface Extractions coupled Directly to Liquid Chromatography for Improving Identification Strategies in Advanced IMS Applications**; Daniel Ryan^{1,2}; David Nei^{2,3}; Boone Prentice^{2,3}; Jeffrey Spraggins^{1,2,3}; Richard Caprioli^{1,2,3,4,5}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁵Department of Medicine, Vanderbilt University, Nashville, TN
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- ThP 285 **Multimodal Imaging Combining Mass Spectrometry and Vibrational Spectroscopy Using a Single Tissue Section and an Integrated Data Processing Workflow;** Rico Scheier¹; Nicolas Desbenoit¹; Jasmin Kniese¹; Heinar Schmidt¹; Andreas Roempp¹; ¹Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth
- ThP 286 **Rapid Quantitation of NNK and NNAL in Rat Urine Using Ultra- Fast Liquid Chromatography Mass Spectrometry;** Estatira Sepehr¹; Matthew S. Bryant¹; ¹Division of Biochemical Toxicology, National Center for Toxicological Research, U.S Food and Drug Administration, Jefferson, AR

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- ThP 288 **Quantitation of Endogenous Small Molecules in Different Tumor Models Using Mass Spectrometry Imaging: Fundamental and Practical Aspects;** John G. Swales^{1,2}; Anna Nilsson³; Gregory Hamm¹; Nicole Strittmatter¹; Christopher Hardy¹; Per E. Andren³; Malcolm R Clench²; Richard J. A. Goodwin¹; ¹Astrazeneca, Cambridge, UK; ²Sheffield Hallam University, Sheffield, UK; ³Uppsala University, Uppsala, Sweden
- ThP 289 **Direct Drug Analysis in Polymeric Implants using DESI Mass Spectrometry Imaging (MSI);** Elizabeth E. Pierson¹; William P. Forrest¹; Megan Mackey¹; Roy Helmy¹; Anthony J. Midey²; Hernando J. Olivios²; Bindesh Shrestha²; ¹Merck Research Laboratories, Rahway, NJ; ²Waters Corporation, Beverly, MA
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- ThP 291 **MALDI Imaging Mass Spectrometry Detection of Intraperitoneally Injected Dipeptide, ZP1609;** Jasmine S.-H. Wang¹; John F. Bechberger²; Moises Freitas-Andrade²; Christian C. Naus²; Shawn N. Whitehead¹; Ken K.-C. Yeung¹; ¹University of Western Ontario, London, ON, Canada, Canada; ²University of British Columbia, Vancouver, BC, Canada
- ThP 292 **Understanding Drug Deposition and Safety in Lung by Mass Spectrometry Imaging;** Gregory Hamm¹; Erica Bäckström²; Tania Baccaga²; Anna Nilsson³; Steven Oag²; Nicole Strittmatter¹; Britta Bonn²; Per E. Andren³; Hui Zhang²; Markus Fridén²; Richard J. A. Goodwin¹; ¹AstraZeneca R&D, Cambridge, UK; ²AstraZeneca R&D, Gothenburg, Sweden; ³Uppsala University, Uppsala, Sweden
- ThP 293 **MALDI Mass Spectrometry Imaging of Therapeutic Monoclonal Antibody in Multicellular Tumor Spheroids (MCTS);** Xin Liu¹; Jessica K. Lukowski¹; Colin Flinders²; Shannon Mumenthaler²; Amanda B. Hummon¹; ¹University of Notre Dame, Notre Dame, IN; ²University of Southern California, Los Angeles, California
- ThP 294 **Diagnosis of Aggregation in Pharmaceutical Preparations by Laser Ablation Electrospray Ionization Mass Spectrometry Imaging;** Patrick A McVey¹; Katherine-Jo Galayda¹; Gregory K. Webster²; Robert S. Houk¹; ¹Iowa State University, Ames, IA; ²AbbVie, North Chicago, IL
- ThP 295 **Dissecting Drug Induced Toxicity of the Murine Olfactory System with Imaging Mass Microscope;** Takuya Tomono¹; Yuki Nakagawa¹; Yudai Tsuji¹; Nobuto Kakuda¹; Tomoyuki Nakamura²; Masaya Ikegawa¹; ¹Doshisha University, Kyotanabe, Japan; ²Kansai Medical University, Hirakata, Japan
- ThP 296 **MSI Analysis of Changes in the Lungs as a Result of Inhaled Drug Dosing;** Alexander Dexter¹; Rory T Steven¹; Alan M Race¹; Adam J Taylor¹; Aateka Patel²; Lea Ann Dailey^{2,3}; Josephine Bunch¹; ¹National Physical Laboratory, Teddington, UK; ²King's College London, London, London; ³für Pharmazeutische Technologie und Biopharmazie Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany
- ThP 297 **Proteomics and Substrate Based MS Imaging of Xenobiotic Metabolising Enzymes in ex vivo Human Skin and a Human Skin Model ;** Narciso Couto¹; Jill Barber¹; Richard Bojar²; James Sidaway³; Malcolm Clench⁴; ¹University of Manchester, Manchester, UK; ²Innovenn Ltd, York, UK; ³Phenotox Ltd, Bollington, UK; ⁴Sheffield Hallam University, Sheffield, S Yorks
- ThP 298 **DESI MS Imaging of Xenobiotic Drugs and Metabolites Using Q-ToF and Tandem Quadrupole Mass Spectrometers for Pharmaceutical Development;** Philippa J. Hart¹; Emmanuelle Claude¹; Emrys Jones¹; Mark W Towers¹; ¹Waters Corporation, Wilmslow, UK
- ThP 299 **Combining Imaging Modalities to Evaluate the Spatial Distributions of SHIV and Antiretroviral Therapies in Putative Viral Reservoirs;** Elias Rosen¹; Claire Deleage²; Nicole White¹; Craig Sykes¹; Lourdes Adamson³; Michelle Mathews¹; George Fedorow¹; Jacob D. Estes²; Paul Luciw³; Angela Kashuba¹; ¹University of North Carolina, Chapel Hill, NC; ²Frederick National Laboratory for Cancer Research, Frederick, MD; ³University of California, Davis, Davis, CA
- ThP 300 **Metabolomic Mapping of Mouse Thymus with Imaging Mass Microscope;** Yudai Tsuji¹; Nobuto Kakuda¹; Hideshi Fujiwaka²; Tomoyuki Nakamura³; Masaya Ikegawa¹; ¹Doshisha University, Kyotanabe, Japan; ²Shimadzu Corporation, Kyoto, Japan; ³Kansai Medical University, Hirakata, Japan
- ThP 301 **Improvement of the Ionization Efficiency of MALDI Using Zeolite Matrix for Simultaneous Imaging of Multiple Drugs Administered in Cancer Cells;** Shusei Nomura¹; Hisanao Hazama¹; Yasufumi Kaneda²; Tatsuya Fujino³; Kunio Awazu^{1,4,5}; ¹Graduate School of Engineering, Osaka University, Suita, Japan; ²Graduate School of Medicine, Osaka University, Suita, Japan; ³Graduate School of Science and Engineering, Toyo University, Kawagoe, Japan; ⁴Graduate School of Frontier Biosciences, Osaka University, Suita, Japan; ⁵Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan
- ThP 302 **Assessing Tissue Region Specific Analyte Suppression in MALDI and DESI Mass Spectrometry Imaging Using Novel Segmentation Based Normalisation Methods;** Adam J Taylor¹; Alex Dexter¹; Kenneth N Robinson^{1,2}; Josephine Bunch¹; ¹National Physical Laboratory, Teddington, Middlesex; ²University of Nottingham, School of Pharmacy, Nottingham, UK
- ThP 303 **Monitoring the Effects of Gene Therapy in a Murine Model of GM1 Gangliosidosis by MALDI Imaging Mass Spectrometry;** Khaja Muneeruddin¹; Bindesh Shrestha²; Hernando J. Olivios²; Sophia Todeasa¹; Eleonora D'Ambrosio¹; Miguel Sena-Esteves¹; Scott A. Shaffer¹; ¹University of Massachusetts Medical School, Worcester, MA; ²Waters Corp, Milford, MA



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- ThP 305 **Submicron Imaging of Intact High Mass Biomolecules Using High Energy Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS);** Hua Tian¹; Louis Sparvero²; Andrew A. Amoscato²; Valerian E. Kagan²; Hulya Bayir²; Nicholas Winograd¹; ¹Pennsylvania State University, State College, PA; ²University of Pittsburgh, Pittsburgh, PA
- ThP 306 **Estimation of Desvenlafaxine in Human K2EDTA Plasma Using LC-MS/MS;** Kolli Narendra Kumar Reddy¹; Srinath Nissankararao²; ¹Vikas Group of Institutions, Vijayawada, India; ²Sri Siddhartha Pharmacy College, Nuzvid, India

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- ThP 308 **IntelliXtract 2.0: Simplified Intelligent Component Extraction and Detection;** Anne Marie Smith¹; Richard Lee¹; Vitaly Lashin¹; Andrey Paramonov¹; ¹ACD/Labs, Toronto, ON, Canada
- ThP 309 **Accurate Deconvolution of Perfectly Coeluting Analytes by Exploiting Differential Expression across Samples;** Kevin Siek¹; David La Fleur¹; Jihong Wang¹; Peter Willis¹; ¹LECO Corporation, Saint Joseph, MI
- ThP 310 **Data-Dependent Scoring Parameter Optimization Using a Spectrum Quality Filter;** Hyunjin Jo¹; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea
- ThP 311 **Latent Group LASSO Regression to Deconvolve Mixture Spectra from Data-Independent Acquisition for Peptide Identification;** Alex Hu¹; William S Noble^{1,2}; Alejandro Wolf-Yadlin^{1,2}; ¹University of Washington Genome Sciences, Seattle, WA; ²University of Washington Computer Science and Engineering, Seattle, WA
- ThP 312 **in silico Validation of Tumor Proteogenomic Annotations;** Anindya Bhattacharya¹; Vineet Bafna¹; ¹University of California, San Diego, La Jolla, CA
- ThP 313 **MSstatsQC: Longitudinal System Suitability Monitoring and Quality Control for Targeted Proteomic Experiments;** Eralp Dogu¹; Sara Mohammed-Taheri²; Susan E Abbatiello³; Micheal Bereman⁴; Brendan MacLean⁵; Birgit Schilling⁶; Olga Vitek²; ¹Mugla University, Mugla, Mugla; ²Northeastern University, Boston, MA; ³Broad Institute, Cambridge, MA; ⁴North Carolina State University, Raleigh, NC; ⁵University of Washington, Seattle, WA; ⁶Buck Institute for Research on Aging, Novato, CA
- ThP 314 **MODplus: Towards the Comprehensive Analysis of Post-Translational Modifications in Shotgun Proteomics;** Seungjin Na¹; Jihyung Kim²; Eunok Paek²; ¹University of California, San Diego, La Jolla, CA; ²Hanyang University, Seoul, South Korea
- ThP 315 **Ultra Deep/High Coverage Proteome Data Raises New Challenges for Protein Inference;** Simon Davis¹; Philip Charles¹; Benedikt M Kessler¹; Roman Fischer¹; ¹University of Oxford, UK, Oxford, Oxfordshire
- ThP 316 **Metrics for Evaluation of Spectral Similarity and Quantitation of Heterogeneity in Mass Spectrometry Data;** Spencer A Thomas¹; Rory T Steven¹; Alan M Race¹; Alexander Dexter¹; Adam J Taylor¹; Santosh Tirunagari²; Ian S Gilmore¹; Josephine Bunch¹; ¹National Physical Laboratory, Teddington, UK; ²University of Surrey, Guildford, UK
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Krzysztof Łacki¹; Błażej Miasojedow¹; Frederik Lermyte²; Dirk Valkenburg^{2,3}; Frank Sobott^{2,4}; Anna Gambin¹; ¹Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warszawa, Poland; ²University of Antwerp, Antwerp; ³Hasselt University, Diepenbeek, Limburg; ⁴University of Leeds, Leeds, Yorkshire

- ThP 318 **Peptide Collision Cross Section Predictor: Rapid Correlation of Ion Mobility Mass Spectrometry Signal with Analyte Structures via Machine Learning;** Xueqin Pang¹; Zichuan Tian²; David Page^{3,4}; Lingjun Li^{1,2}; ¹School of Pharmacy, University of Wisconsin Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin Madison, Madison, WI; ³Department of Biostatistics and Medical Informatics, University of Wisconsin-Madison, Madison, WI; ⁴Department of Computer Sciences, University of Wisconsin-Madison, Madison, WI
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- ThP 320 **Intensity-dependent Mass Search in Liquid Chromatography Mass Spectrometry Based Metabolomics;** Yunong Li¹; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada
- ThP 321 **MORESSA: An Ensemble Methodology for Simultaneous MS/MS Spectral Similarity Searching and Structure Elucidation;** Tytus D. Mak¹; Stephen E. Stein¹; ¹National Institute of Standards & Technology, NIST, Gaithersburg, MD
- ThP 322 **Monoclonal Antibody de novo Sequencing by Deep Learning;** Hieu Tran¹; Xianglilan Zhang¹; Lei Xin²; Lin He²; Baozhen Shan²; Ming Li¹; ¹University of Waterloo, Waterloo, ON, Canada; ²Bioinformatics Solutions Inc, Waterloo, ON, Canada
- ThP 323 **Compositional Proteomics: Utilizing Simplicial Regression to Enhance Protein Detection and Estimation in Multiplexed Experiments;** Jonathon O'Brien¹; Joao Paulo¹; Christopher Rose¹; Steve Gygi¹; ¹Harvard Medical School, Boston, MA
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- ThP 325 **Single-Molecule Protein Identification by Nanopore Sensors;** Mikhail Kolmogorov¹; Eamonn Kennedy²; Zhuxin Dong²; Gregory Timp²; Pavel Pevzner¹; ¹Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; ²Electrical Engineering and Biological Science, University of Notre Dame, Notre Dame, USA
- ThP 326 **Flexible Library Assisted Search (FLASH): a Hybrid Library/Database Search Engine for Proteomics;** Joon-Yong Lee¹; Grant M Fujimoto¹; Christopher S Wilkins¹; Richard Smith¹; Sam Payne¹; ¹Pacific Northwest National Lab, Richland, WA
- ThP 327 **Themis: Batch Pre-Processing for Ultrahigh Resolution Complex Mixture Data;** Remy Gavard¹; David Rossell^{1,2}; Simon E F Spencer¹; Mark P Barrow¹; ¹University of Warwick, Coventry, UK; ²Universitat Pompeu Fabra, Barcelona, Spain
- ThP 328 **Detection of Differentially Abundant Proteins with MSstats 3.6 Improves Reproducibility between Data Processing Tools;** Meena Choi¹; Eduard Sabido²; Oliver M. Bernhardt³; Nicholas Shulman⁴; Brendan MacLean⁴; Olga Vitek⁵; ¹Northeastern University, Boston, MA; ²Center for Genomics Regulation, Barcelona, Spain; ³Biognosys, Zurich, Switzerland; ⁴University of Washington Genome Sciences, Seattle, WA; ⁵Northeastern University, Boston, MA



- ThP 329 **Novel Approach for Chemical Formula Identification Based on Isotopic Distribution Observed with Ultrahigh Resolution FTICR Mass Spectrometer**; Evgeny Zhvansky¹; Anatoly Sorokin¹; Igor Popov¹; Vsevolod Shurhkhay²; Nikita Levin¹; Alexander Potapov²; Eugene (Evgeny) Nikolaev^{1,3,4}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ³Skolkovo institute of science and technology, Skolkovo, Russia; ⁴Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia
- ThP 330 **The “Mechanical Mass Spectrometrists”, or: How to Collect 100,000 Manual Peak Annotations**; Manor Askenazi¹; Johannes Graumann^{2,3}; Hisham Ben Hamidane²; Anja M. Billing²; Rudolf Engelke²; Sara E. Lendal²; Sunkyu Choi²; ¹Biomedical Hosting LLC, Arlington, MA; ²Weill Cornell Medicine - Qatar, Doha, Qatar; ³Max Planck Institute for Heart and Lung Research, Bad Nauheim, Germany
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- ThP 334 **The Database for Mining Biomarkers in the Brain Tumor Tissue Mass-Spectra**; Anatoly Sorokin¹; Vsevolod Shurhkhay²; Igor Popov¹; Evgeny Zhvansky¹; Nikita Levin¹; Alexander Potapov²; Eugene (Evgeny) Nikolaev^{1,3,4}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ³Skolkovo institute of science and technology, Skolkovo, Russia; ⁴Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia
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- ThP 336 **New Peak Finding and Integration Algorithms in Skyline**; Nicholas Shulman¹; Max Horowitz-Gelb¹; Andreas F Tillack²; Michael H Gelb²; Bruce H Robinson²; Brendan MacLean¹; ¹University of Washington Genome Sciences, Seattle, WA; ²Department of Chemistry, University of Washington, Seattle, WA
- ThP 337 **MilkyWay: A Galaxy Platform for Quantitative Comparative Analysis of Bottom-Up Proteomic Mass Spectrometry Datasets**; William D Barshop¹; Hee Jong Kim¹; James Akira Wohlschlegel¹; ¹University of California Los Angeles, Los Angeles, CA
- ThP 338 **pClean: A Powerful Filtration to Remove the Uninformative Signals in MS Spectra for Peptide Identification**; Yamei Deng^{1,2}; Bo Wen²; Shaoxing Xu²; Lin Wu¹; Yan Ren²; Siqi Liu²; ¹Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; ²BGI-Shenzhen, Shenzhen, China
- ThP 339 **ProSight Annotator: Freeware for the Generation of UniProt Formatted XML Files Containing Custom User-Specified Features**; Joseph B Greer¹; Ryan T. Fellers¹; Richard D. LeDuc¹; Bryan P. Early¹; Alexandra J. VanNispen¹; Paul M. Thomas¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
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- ThP 342 **Exploring Multiple Independent Variables Associated with Large Proteomics and Metabolomics Datasets Using a Flexible Hierarchical Organization scheme**; Phillip Seitzer¹; Seth Just¹; Susan Ludwigsen¹; Jacob Lippincott¹; Caleb Emmons¹; Nick Vincent-Maloney¹; Jimar Miller¹; Brian Searle^{1,2}; ¹Proteome Software, Portland, OR; ²University of Washington, Seattle, WA
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- ThP 349 **GiaPronto: A One-Click Online Data Analysis and Visualization for Proteomics**; Amber K. Weiner^{1,2,3}; Simone Sidoli¹; Sharon J. Diskin^{2,3}; Benjamin A. Garcia^{1,3}; ¹Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; ²Division of Oncology, Department of Pediatrics, Children's Hospital of Philadelphia, Philadelphia, PA; ³Genomics and Computational Biology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- ThP 350 **MassBank of North America: An Open Access Metadata-Centric, Auto-Curating Repository for Mass Spectra from Different Instrument Platforms**; Gert Wohlgemuth¹; Sajjan S. Mehta²; Oliver Fiehn¹; ¹UC Davis, Davis, CA; ²University of California, Davis, Davis, CA

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- ThP 358 **The Implications of Detector Performance in GC/MS and LC/MS Analysis – Detectors Make the Difference!;** Nathan Contino¹; Jeff Kernan¹; Harry Prest¹; Bjorn Flatt¹; Bill Russ¹; ¹*Agilent Technologies Inc., Santa Clara, CA*
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- ThP 362 **Ultra High Resolution MS Aids Unknown Extractable Component Identification;** Kate Comstock¹; Seema Sharma¹; Jesse D. Canterbury¹; Vlad Zabrouskov¹; ¹*Thermo Fisher Scientific, San Jose, CA*
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- ThP 364 **Development of a Ultrahigh Resolution Multi-reflection Time-of-Flight Mass Spectrometer for Native Mass Spectrometry;** Keyong Hou¹; Ping Chen¹; Jichun Jiang¹; Haiyang Li¹; ¹*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*
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- ThP 366 **A Modular Ion Funnel for Improved Sensitivity in Proton-Transfer-Reaction – Time-Of-Flight Mass Spectrometry (PTR-TOFMS) Instruments;** Alfons Jordan¹; Christian Lindinger¹; Stefan Feil¹; Paul Mutschlechner¹; Gernot Hanel¹; Eugen Hartungen¹; Jens Herbig¹; Lukas Maerk¹; Philipp Sulzer¹; Simone Juerschik¹; ¹*IONICON Analytik GmbH, Innsbruck, Austria*
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- ThP 368 **Coaxial Surface Induced Dissociation of Mass-Selected Ions;** Xinwei Liu¹; Xiaoyu Zhou¹; Zheng Ouyang^{1,2}; ¹*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China;* ²*Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN*
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- ThP 372 **Comprehensive Modeling and Experimental Validation of Ultrahigh Mass Resolution Linear Time-Of-Flight Mass Spectrometry;** Yu-Meng Ou^{1,2}; Yin-Hung Lai¹; Yi-Hong Cai¹; Chih-Hao Hsiao¹; Cheng-Kai Jan¹; Huan-Tsung Chang²; Yi-Sheng Wang¹; ¹*Genomics Research Center Academia Sinica, Taipei;* ²*Department of Chemistry, National Taiwan University, Taipei, Taiwan*
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- ThP 377 **Analyzing Large Protein with High Resolution by AMS-200 series: inTrap MALDI Mass Spectrometer;** Shih-Chieh Yang¹; Szu-Wei Chou¹; Yao-Hsin Tseng¹; Yi-Kun Lee¹; Chih-kuang Chen¹; Chun-Yen Cheng¹; ¹*AcroMass technologies, Inc., Taipei*
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- ²OiArna LLP, Almaty, Kazakhstan; ³Nazarbayev University, Astana, Kazakhstan
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- ThP 389 **New FAIMS with Heated Electrospray Ionization (HESI) Source for High Chromatographic Flow Rate Application**; Satendra Prasad¹; Michael Belford²; Rae Ana Snyder²; Susan E. Abbatiello³; Jean-Jacques Dunyach⁴; ¹Thermo Fisher Scientific, San Jose, CA; ²ThermoFisher Scientific, San Jose, CA; ³Thermo Scientific, Cambridge, MA; ⁴Thermo Fisher Scientific, San Jose, CA
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- ThP 391 **Strategies for Improving FAIMS Performance for Clinical Applications**; Michael Wei¹; Robin H.J. Kemperman¹; Michael Costanzo²; Jared Boock³; Richard A. Yost¹; ¹University of Florida, Gainesville, FL; ²Breathtec Biomedical, Inc., Gainesville, Florida; ³Cannabix Technologies, Gainesville, Florida
- ThP 392 **Mitigating Fragmentation of Peptides with Controlled Clustering**; J.C. Yves Leblanc¹; Brendon Seale^{1,2}; Bradley B. Schneider¹; Aaron Wheeler²; ¹SCIEX, Concord, ON, Canada, ON, Canada; ²University of Toronto, Toronto, ON, Canada
- ThP 393 **The Impact of Improved Selectivity through Enhanced Resolution and Field Asymmetric Ion Mobility on Defined Method LOQs and LODs**; Hans Schweingruber¹; Michael Belford¹; Satendra Prasad¹; Susan E. Abbatiello¹; Claudia Martins¹; Nelson Wijeratne¹; Mary Blackburn²; ¹ThermoFisher, San Jose, CA; ²Thermo Fisher Scientific, San Jose, CA
- ThP 394 **APPI-FAIMS-FTMS for the Investigation of Structural Features of Isomeric Crude Oil Constituents**; Alessandro Vetere¹; Wolfgang Schrader²; ¹Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; ²Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr
- ThP 395 **How Mass Spectrometer Model and Electrode Temperature Determines FAIMS Separation**; Michael Belford¹; Satendra Prasad¹; Susan E. Abbatiello²; Hoa Pham¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Scientific, Cambridge, MA
- ThP 396 **Exploring the Separation of Phospholipids Using a Novel FAIMS Device in Conjunction with MS/MS Mode of Analysis**; Rae Ana Snyder¹; Satendra Prasad¹; Michael Belford¹; ¹Thermo Fisher Scientific, San Jose, California
- ThP 397 **Pre-Filtration of Transition Metals in Differential Mobility Spectrometry**; Ifeoluwa Ayodeji¹; Theresa Evans-Nguyen¹; Ronelle Bailey¹; Christina Mancuso¹; ¹University of South Florida, Chemistry department, Tampa, FL
- ThP 398 **Separation of Triacylglycerol Positional Isomers in Plants Using Differential Mobility Spectrometry**; Jesse Balcer¹; Jeffrey Gilbert²; Laura Wayne²; Yelena Adelfinskaya²; Scott Greenwalt²; Daniel Gachotte²; Lisa Buchholz²; ¹Dow AgroSciences, Indianapolis, IN; ²Dow AgroSciences, Indianapolis, IN
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- ThP 399 **Influence of Ionization Source Conditions on the Protomer Population Distribution of Anilinium and Related Cations**; Hanxue Xia; SIT, jersey city, New Jersey
- ThP 400 **Towards Serpentine Ultra Long Ion Path for Enhanced Resolution Using Traveling Wave Structures for Lossless Ion Manipulations (SUPER TW-SLIM)**; Ahmed Mohamed Hamid¹; Sandilya V.B. Garimella¹; Yehia M Ibrahim¹; Liulin Deng¹; Aneesh Prabhakaran¹; Ian K Webb¹; Gordon A Anderson¹; Spencer A Prost¹; Randolph V Norheim¹; Jeremy A Sandoval¹; Colby E Schimelfenig¹; Erin S Baker¹; Richard D. Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA
- ThP 401 **Evaluation of Pulsed Nano-ESI Atmospheric Pressure Ion Mobility MS for Collision Cross Section Measurements**; William McMahon¹; Rohan Dalvi²; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC; ²Montgomery Blair High School, Silver Spring, MD



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- ThP 402 **Supercritical Planar DMA P5 working at a resolving power of 110**; Mario Amo González¹; Juan Fernandez de la Mora²; ¹SEADM, Boecillo, Spain; ²Yale University, New Haven, Connecticut
- ThP 403 **Structural Specificity of Ion Mobility Collision Cross Section for Characterization of Lipids**; Jody C. May¹; Stacy D. Sherrod¹; Katrina L Leaptrot¹; Charles M. Nichols¹; John A. McLean¹; ¹Center for Innovative Technology, Vanderbilt University, Nashville, TN
- ThP 404 **Simultaneous and Co-located Dual Polarity Ion Confinement and Separation in Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)**; Isaac K. Attah¹; Sandilya V.B. Garimella²; Yehia M. Ibrahim²; Ian K. Webb²; Aneesh Prabhakaran²; Richard D. Smith²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA
- ThP 405 **Development of Ion-Mobility Orbitrap for Analysis of Large Proteins and Protein Complexes**; Michael Poltash¹; David H Russell¹; ¹Texas A&M University, College Station, Texas
- ThP 406 **Ion Mobility Spectrometry of Foldamers and Foldaxanes. Optimization of Parameters Used for Theoretical CCS Calculation**; Frederic Rosu¹; Yann Ferrand¹; Victor Maurizot¹; Ivan Huc¹; Valérie Gabelica^{2,3}; ¹CNRS / Univ. Bordeaux, Pessac, France; ²University of Bordeaux, Pessac, FR; ³Inserm, Bordeaux, France
- ThP 407 **An Ion Mobility filter based on Structures for Lossless Ion Manipulations (SLIM)**; Aneesh Prabhakaran¹; Ahmed Mohamed Hamid²; Yehia M Ibrahim²; Sandilya Garimella²; Robert G Ewing²; Blandina R Valenzuela²; Jeremy A Sandoval²; Richard D. Smith²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA
- ThP 408 **Collision Cross Section Measurement in Traveling Wave Ion Mobility Spectrometry: Analytical Comparison of Functions for Fitting Calibration Curves**; Alana L Rister¹; Abby S Gelb¹; Eric D Dodds¹; ¹University of Nebraska - Lincoln, Lincoln, NE
- ThP 409 **Correlating Resolving Power, Resolution, and Collision Cross Section: A Cross Platform Study of Separation Efficiency in Ion Mobility Spectrometry**; James Dodds¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- ThP 410 **Collision Cross Section Calibration with Structures for Lossless Ion Manipulations Mixture Analysis by Traveling Wave Ion Mobility**; Ian K. Webb¹; Liulin Deng¹; Ahmed M Hamid¹; Roza Wojcik¹; Erin S Baker¹; Yehia M Ibrahim¹; Richard D. Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA
- ThP 411 **Selective Ion-Neutral Clustering to Enhance Ion Mobility Separation Factors**; Pearl Kwantwi-Barima; Washington State University, Pullman, WA
- ThP 412 **Optimization of Electron Capture Dissociation for the Analysis of Glycans, Peptides, and Proteins Using a IM-QTOF Mass Spectrometer**; James A. Hill¹; Rebecca S. Glaskin¹; Valery G. Voinov²; Joseph S. Beckman²; Catherine E Costello¹; ¹Boston University School of Medicine, Boston, MA; ²e-MSion, Corvallis, OR
- ThP 413 **Accurate Absolute Collision Cross Sections via the "CRAFTI" FTICR Linewidth Technique**; Anupriya Anupriya¹; Elaura Gustafson¹; David V. Dearden²; ¹Brigham Young University, Provo, UT; ²Brigham Young University, Provo, UT
- ThP 414 **Determining the Upper-Mass Limit for Obtaining Accurate CRAFTI Collision Cross Section Measurements Using Variable Length Polyalanine Peptides**; Brigham Pope¹; David V. Dearden¹; Anupriya Anupriya¹; ¹Brigham Young University, Provo, UT
- ThP 415 **Identification of Isomers by Fingerprint Isotopic Fine Structure in High-Resolution FAIMS Spectra**; Julia L. Kaszycki¹; Matthew A. Baird¹; Andrew P. Bowman¹; Alexandre Shvartsburg²; ¹Wichita State University, Wichita, KS; ²Wichita State University, Wichita, KS
- ThP 416 **Exploring Dendrimers as Calibrants for Ion Mobility-Mass Spectrometry**; Scott M. Grayson¹; Michael Malkoch^{2,3}; Jamie Godfrey³; Surintra Mongkhontreerat³; Nick Tomczyk⁴; Jakub Ujma⁴; Kevin Giles⁴; ¹Tulane University, New Orleans, LA; ²KTH Royal Institute of Technology, Stockholm, Sweden; ³Polymer Factory Sweden AB, Stockholm, Sweden; ⁴Waters Corp., Wilmslow, UK
- ThP 417 **Conformational Dynamics in Ion Mobility Data**; Poyer Salomé¹; Comby-Zerbino Clothilde²; Choi Chang Min²; MacAleese Luke²; Salpin Jean-Yves¹; Dugourd Philippe²; Fabien Chiro³; ¹LAMBE, Université Evry Val d'Essonne, CEA, CNRS, Université Paris-Saclay, Evry, France; ²Institut Lumière Matière, Université de Lyon, Université Lyon 1, CNRS, Lyon, France; ³Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France
- ThP 418 **Quantitative Ion Mobility-Mass Spectrometry for Identifying Protein/Peptide Conformation/Multimer Ions**; KENT GILLIG¹; Chung-Hsuan Chen¹; ¹Academia Sinica, Taipei, Nankang, Section 2, Taipei 115
- ThP 419 **Collision Cross Sections of Polyoxometalates : Linking Experimental and Theoretical Values**; Sébastien Hupin¹; Hélène Lavanant¹; Madeleine Piot²; Guillaume Izet²; Carlos Afonso¹; ¹Normandie Univ., UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France; ²Institut Parisien de Chimie Moléculaire UMR CNRS 8232, Sorbonne Universités, UPMC-Paris 6, 4 Place Jussieu, 75005 Paris, France
- ThP 420 **New Developments in Gated Trapped Ion Mobility Spectrometry for Coupling with FT-ICR Mass Analyzers**; Mark Ridgeway¹; Mel Park¹; ¹Bruker Daltonics Inc., Billerica, MA
- ThP 421 **True vs. Average Mobility. New developments in Ion Mobility Separation**; Carlos Larriba Andaluz¹; Tianyang Wu²; ¹IUPUI, Indianapolis, IN; ²IUPUI, Indianapolis, IN
- ThP 422 **A Comparison of Collision Cross Section Calibrants for Traveling Wave Ion Mobility Spectrometry Reveals Significant Discrepancies between Molecular Classes**; Eric D. Dodds¹; Alana L. Rister¹; Abby S. Gelb¹; ¹University of Nebraska - Lincoln, Lincoln, NE

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- ThP 423 **Improving Routine Analysis of Glycan Profiles in a QC Environment Using Spectral Libraries**; Brooke M. Koshel¹; Ximo Zhang¹; Robert Birdsall¹; Joe Fredette¹; Min Du¹; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA
- ThP 424 **High-Throughput Comprehensive Analysis of Trace D- and L- Amino Acids Using Extra-Facile Chiral Separation and Column Switching**; Yuki Uno¹; Toshikazu Minohata¹; Jun Watanabe¹; Hidetoshi Terada^{1,2}; Junko Iida^{1,2}; Yosuke Nakano³; Eiichiro Fukusaki^{2,3}; ¹Shimadzu Corporation, Kyoto, Japan; ²Osaka University Shimadzu Analytical Innovation Research Laboratory, Graduate School of Engineering, Osaka University, Suita, Japan; ³Department of Biotechnology, Graduate School of Engineering, Osaka University, Suita, Japan
- ThP 425 **Open Data Standard for LC/MS Data, Methods, and Results**; David Peterson¹; Heiko Fessenmayr²; ¹Agilent Technologies Inc., Santa Clara, California; ²Agilent Technologies, Inc., Santa Clara, CA
- ThP 426 **Taking Nano Liquid Chromatography Coupled to Mass Spectrometry One Step Closer to the Clinics**; Ole Kristian Brandtzaeg¹; Meire Ribeiro da Silva^{1,2}; Tore Vehus¹; Hanne Roberg-Larsen¹; Elsa Lundanes¹; Steven Ray



- Wilson¹; ¹University of Oslo, Oslo, Oslo; ²Universidade de São Paulo - USP, Sao Paulo, Brazil
- ThP 427 **Determination of Isoflavones in Dietary Supplements: a Comparison of Mass Detection with UV Detection;** Jinchuan Yang¹; Mark Benvenuti¹; Kenneth Rosnack¹; Ramesh P Rao²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK
- ThP 428 **High-Throughput Strategies for Label-Free and SILAC LC-MS/MS Proteomics;** Yuan-wei David Nei¹; Rey Redha¹; Carrie E. Romer¹; Jamie L. Allen²; Danielle B. Gutierrez²; Tina Tsui²; Michael R Heaven³; Jeremy L. Norris²; Richard M. Caprioli²; ¹MSRC Vanderbilt University, Nashville, TN; ²MSRC Vanderbilt University, Nashville, TN; ³Vulcan Analytical, LLC, Birmingham, AL
- ThP 429 **Discovery Ion Current - A Novel Approach to Plot Total Ion Current Real-Time by Enhancing Signal from Newly Detected Ions;** Lawrence Klecha¹; Daniel Eikel¹; ¹Advion Inc., Ithaca, NY
- ThP 430 **Selectivity Comparison of BromoBenzyl(PBr) to FluoroPhenyl(PFP) Core-Shell HPLC Columns;** Ken Tseng¹; Toshi Ono¹; Tsunehisa Hirose²; ¹Nacalai USA, San Diego, CA; ²Nacalai Tesque, Kyoto, Japan
- ThP 431 **How Combined New Approaches Can Improve Quantitative and Qualitative LC-MS;** Stephan Altmair¹; Hans Griesinger¹; Michael Schulz¹; ¹Merck KGaA, Darmstadt, Germany
- ThP 432 **Spectrum Evaluation for the 2017 Released NIST Tandem MS Library;** Yuxue Liang¹; Pedatsur Neta²; Xiaoyu Yang²; Stephen E Stein²; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²National Institute of Standards and Technology, Gaithersburg, MD
- ThP 433 **Measurement of Amino Acid Modification after Fast Photochemical Oxidation of Proteins Utilizing Online Low-Flow Size Exclusion Chromatography;** Sandeep K Misra¹; Joshua S. Sharp¹; ¹University of Mississippi, Oxford, MS
- ThP 434 **Chromatographic Behaviour of PTM-Carrying Peptides in Proteomic Experiments (RPLC, HILIC, CZE);** Vic Spicer¹; Haley Neustaeter¹; Evelyn Ang¹; Ying Lao¹; Helene Perreault¹; Oleg V. Krokhin²; ¹University of Manitoba, Winnipeg, MB; ²University of Manitoba, Winnipeg, MB
- ThP 435 **Automated Targeted Screening of Leachables in Pharmaceutical Drug Products by Single Quadrupole Mass Spectrometer System;** Syed Salman Lateef¹; Siji Joseph¹; ¹Agilent Technologies India, Bangalore, India
- ThP 436 **Method for Quick and Efficient Packing of 50 cm Capillary Liquid Chromatography Columns for Mass-Spectrometry Based Proteomics;** Sergey I. Kovalchuk¹; Wojciech Michalak¹; Adelina Rogowska-Wrzesinska¹; Ole N. Jensen¹; ¹Univ. Southern Denmark, Odense, Denmark
- ThP 437 **Eliminating a Common Yet Obscure Noise Source in LCMS and ICPMS ;** Robert Cunico¹; Michael J Pinkerton¹; Steve Graham¹; ¹ASI, Inc., Richmond, CA
- ThP 438 **2D-LC/MS Analysis of Fosfomycin Trometamol and Related Substances in Stress Testing Solvent;** Nan Hu¹; Xialong Zuo¹; ¹Agilent Technologies, Beijing, China
- ThP 439 **Revealing Hidden Impurities in Bio-Pharmaceuticals by Multi-Dimensional Chromatography Preceding ESI-MS;** Stephan Buckenmaier¹; Dwight Stoll²; Patrik Petersson³; ¹Agilent, Waldbronn, Baden-Wuerttemberg; ²Gustavus Adolphus College, Saint Peter, MN; ³Novo Nordisk A/S, Måløv, Denmark
- ThP 440 **Toward Rapid Structure Elucidation of Cyclic Peptide Late Stage Functionalization using UPLC-HRMS with Customizable Reaction-Driven Data Processing;** Jason Hoar¹; Fabien Fontaine²; Mikhail Reibarkh¹; Yong Liu¹; Ismael Zamora²; Shane Kraska¹; Christopher Sinz¹; Kevin Bateman¹; ¹Merck & Co., Inc, Rahway, NJ; ²Molecular Discovery, London, UK
- ThP 441 **The Development of a Method for the Determination of Cortisol and 6-Beta-Hydroxycortisol in Human Urine Using 2-D Chromatography;** Jeff Jeppson¹; Elizabeth Dibbern¹; Ridha Nachi¹; Curtis Sheldon¹; ¹Celerion, Lincoln, NE
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- ThP 442 **Accurate Mass and Retention Time Library of Serum Lipids for Type 1 Diabetes Research;** Ngoc Vu¹; Monica Narvaez-Rivas²; Qibin Zhang^{1,2}; ¹University of North Carolina at Greensboro, Greensboro, NC; ²Center for Translational Biomedical Research, Kannapolis, NC
- ThP 443 **Dynamic and Temporal Assessment of Human Dried Blood Spot MS/MSALL Shotgun Lipidomics Analysis;** Fei Gao¹; Justice McDaniel¹; Emily Y Chen¹; Hannah Rockwell¹; Jeremy Drolet¹; Vivek K Vishnudas¹; Vladimir Tolstikov¹; Rangaprasad Sarangarajan¹; Niven R Narain¹; Michael A Kiebish¹; ¹Berg, LLC, Framingham
- ThP 444 **Elongation of Very Long Chain Fatty Acids (ELOVL) Isozymes Activity – A Lipidomics Approach Using Infusion-Based MS/MSALL;** Goncalo Vale¹; Matthew Mitsche¹; Bonne Thompson¹; Kaitlyn Eckert¹; Alex Treacher¹; William Trenfield¹; Young-ah Moon¹; Jeffrey McDonald¹; ¹UT Southwestern, Dallas, TX
- ThP 445 **LC-MS Analysis of Lipids Nanoparticles (LNPs): One Shot, Four Lipids;** Jiang Qian¹; Kanwaldeep Gill¹; Zi Wang¹; ¹GSK Vaccines, Rockville, MD
- ThP 446 **Comparison of Eight High-Resolution LC-MS Platforms Validates Accurate Quantifications in Untargeted Plasma Lipidomics;** Tomas Cajka¹; Jennifer T Smilowitz^{2,3}; Oliver Fiehn¹; ¹NIH West Coast Metabolomics Center, University of California Davis, Davis, CA; ²Department of Food Science and Technology, University of California Davis, Davis, CA; ³Foods for Health Institute, University of California Davis, Davis, CA
- ThP 447 **Development of an Integrated Workflow for Profiling and Semi-Quantitative Analysis of Lipids ;** Sheher Bano Mohsin¹; Kevin Williams²; Durairaj Renu³; Ningombam Sanjib Meitei⁴; Shyam Kalakoti³; Stephen Madden⁵; ¹Agilent Technologies Inc., Wood Dale, IL; ²UCLA, Los Angeles, California; ³Strand Life Sciences, Bengaluru, India; ⁴PREMIER Biosoft, Indore, India; ⁵Agilent Technologies Inc., Santa Clara, California
- ThP 448 **Investigating the Lipidomic Dynamics of Torpor through Examination of Hibernating Squirrel Liver Tissue and Dehydrated Frog Leg Tissue;** Katrin Blank¹; Sam Williamson¹; Hillary Weinert¹; Carlos R. Canez¹; Kenneth Storey¹; Jeffrey C. Smith¹; ¹Carleton University, Ottawa, ON, Canada
- ThP 449 **Structural Characterization of Bioactive Fatty Acid Isomers Using Liquid Chromatography–Differential Mobility Spectrometry and Electron-Induced Dissociation Mass Spectrometry (LC-DMS-EID);** Kazutaka Ikeda^{1,2}; Shuh Yasuda¹; Yuuya Senoo¹; Makoto Arita^{1,2,3}; J. Larry Campbell⁴; J.C. Yves Leblanc⁴; Paul Rs Baker⁵; Takashi Baba⁴; ¹RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; ²Yokohama City Univ., Yokohama, Japan; ³Keio University, Tokyo; ⁴SCIEX, Concord, ON, Canada; ⁵SCIEX, Redwood City, CA
- ThP 450 **Development of a High-Sensitivity Method for Lipidomics of Small Volumes of Biological Fluids by nanoLC-MS;** Adriana Zardini Buzatto¹; Jaspaul Tatlay¹; Brian Kwon²; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada; ²University of British Columbia, Vancouver, BC, Canada
- ThP 451 **Investigation of Brain Tumors by Online Liquid Extraction Combined with ESI Ionization and Ultrahigh Resolution FTICR Mass Spectrometry;** Igor Popov^{1,2,3};

Evgeny Zhvansky¹; Vsevolod Shurhkhay^{1,4}; Nikita Levin¹; Alexey Kononikhin^{1,2}; Anatoly Sorokin¹; Oleg Kharybin⁵; Yuri Kostyukovich^{1,5}; Maria Indeykina^{1,2,3}; Alexander Potapov⁴; Eugene (Evgeny) Nikolaev^{1,2,5}; ¹Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; ²Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; ³Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; ⁴N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; ⁵Skolkovo Institute of Science and Technology, Skolkovo, Russia

ThP 452 **Characterizing Human Meibum by Shotgun Lipidomics, MS/MSall and Successive Polarity Switching**; Jianzhong Chen¹; Kelly K Nichols²; ¹University of Alabama at Birmingham, Birmingham, AL; ²University of Alabama at Birmingham, Birmingham, AL

ThP 453 **Acoustically-induced Electrospray Mass Spectrometry of Extracellular Vesicle Lipids**; Xabier Osteikoetxea¹; Martin Bachman¹; Ian Sinclair¹; Nikki Heath¹; Lois Grant¹; Jonathan Wingfield²; Niek Dekker³; Ross Overman¹; ¹AstraZeneca R&D, Alderley Park, UK; ²AstraZeneca R&D, Cambridge, UK; ³AstraZeneca R&D, Gothenburg, Sweden

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ThP 455 **A Novel LC-MS/MS Method for Ganglioside Profiling of Glaucoma Disease in Mice**; Ashta Lakshmi Prasad Gobburi¹; Denise Inman²; David J Anderson¹; ¹Cleveland State University, Department of Chemistry, Cleveland, OH; ²Northeast Ohio Medical University, Rootstown, Ohio

ThP 456 **Challenges for the Quantification of DMG-PEG GM-020 in Mouse Plasma by HPLC-MS/MS**; Lijuan Fu¹; Bryce Ashby¹; Shawn Burton¹; Qian Guo¹; Scott Reuschel¹; Min Meng¹; Aihua Liu¹; ¹Covance, Salt Lake City, UT

ThP 457 **High Throughput Lipid Identification and Quantification Using a Directed HRAM LC-MS-MS approach on a Modified Quadrupole-Orbitrap Mass Spectrometer**; Reiko Kiyonami¹; David Peake¹; Andreas F. Huhmer¹; ¹ThermoFisher Scientific, San Jose, CA

ThP 458 **Locating Apolipoprotein A2 Protein in the Central Nervous System**; Sausan Azzam^{1,2}; Xiaolin Li^{1,2}; Mark R. Chance^{1,2}; Kingman P. Strohl³; ¹Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; ²Department of Nutrition, Case Western Reserve University, Cleveland, OH; ³Department of Medicine, University Hospitals Case Medical Center, Cleveland, OH

ThP 459 **Development of an HILIC Based LC-MS/MS for High-Throughput Targeted Lipidomics**; Junhua Wang¹; Mackenzie Pearson¹; Paul Rs Baker¹; ¹SCIEX, Redwood City, CA

ThP 460 **Identification and Quantification of Esterified Hepoxilin A3 in the ileum of Mice after Total Body Irradiation Using Oxidative Phospholipidomics**; Yulia Y Tyurina¹; Vladimir A Tyurin¹; Andrew A Amoscato¹; Tami Anthony-muthu¹; Michael W Epperly¹; Simon S Watkins¹; Joel S Greenberger¹; Hülya Bayir¹; Valerian E Kagan¹; ¹University of Pittsburgh, Pittsburgh, PA

ThP 461 **Towards Quantitative Analysis of MALDI Mass Spectral Data Using linear Poisson Independent Component Analysis**; Somrudee Deepaisarn¹; Adam McMahon¹; Neil

A. Thacker¹; Paul D. Tarl¹; Ashley Seepujak¹; ¹University of Manchester, Manchester, UK

ThP 462 **Dysregulated Lipid Profiles of Non-Alcoholic Fatty Liver Disease (NAFLD)**; Timothy J Garrett¹; Rainey E Patterson²; Baljit Ubhi³; Ken Cusi⁴; ¹Univ of Florida, Gainesville, FL; ²Eastman Chemical Company, Kingsport, TN; ³SCIEX, Redwood City, CA; ⁴University of Florida, Gainesville, FL

ThP 463 **Cardiolipin Remodeling in the Developing Brain after Trauma**; Tamil S Anthony-muthu¹; Honglu Chao^{2,3}; Andrew A Amoscato²; Jing Ji³; Valerian E Kagan²; Hülya Bayir²; ¹University Of pittsburgh, Pittsburgh, PA; ²University of Pittsburgh, Pittsburgh, PA; ³Nanjing Medical University, Nanjing, China

ThP 464 **The Unusual Ionization Behavior of Ceramides on Sciex 6500QTRAP Instrument during LC-MS/MS Analyses**; Irina Bronova¹; John Jung¹; Evgeny Berdyshev¹; ¹National Jewish Health, Denver, CO

ThP 465 **Untargeted Metabolomic Analysis of omega-3 Ethyl Ester Supplementation**; Stacy Gelhaus¹; Francisco J. Schopfer¹; Sonia R. Salvatore¹; Carsten Skarke²; ¹Univ of Pittsburgh, Pittsburgh, PA; ²University of Pennsylvania, Philadelphia, PA

ThP 466 **Novel Method for Total Butyrate Quantification in Human Milk Using GC-MS**; Stephanie P. Shu¹; Judy Cundiff¹; Michael Gray¹; Sarah Maria¹; Shay Phillips¹; Ardythe L. Morrow²; ¹Mead Johnson Nutrition, Evansville, IN; ²Cincinnati Children's Hospital Medical Center, Cincinnati, OH

ThP 467 **Contribution of Biosynthesis vs Remodeling to the Diversity of Cardiolipins in Genetically and Nutritionally Manipulated Yeast Cells: Differential LC-MS Assessments**; Vladimir A. Tyurin¹; Yulia Y. Tyurina¹; Wenjia Lou²; Feng Qu¹; Jenney Liu³; Maik Hüttemann³; Dariush Mohammadyani^{1,4}; Michael A. Frasso¹; Peter Wipf¹; Hülya Bayir¹; Miriam L. Greenberg³; Valerian E. Kagan¹; ¹University of Pittsburgh, Pittsburgh, PA; ²Wayne State University, Detroit, MI; ³Wayne State University, Detroit, MI; ⁴Johns Hopkins University, Baltimore, MA

ThP 468 **Diagnostic Evaluation of Steroidomics in a Breast Cancer Cohort in Sweden by Convergence Chromatography-Tandem Mass Spectrometry**; Neil De Kock¹; Kumari Ubhayasekera¹; Jonas Bergquist¹; ¹Uppsala University, Uppsala, Sweden

ThP 469 **Optimization of LC-ESI-MS Methods for Targeted and Semi-Targeted Screening of N-acyl Phosphatidylethanolamines in Mouse Brain Tissue**; Theresa McLaughlin¹; Ludmila Alexandrova²; Allis Chien²; ¹Stanford University, Palo Alto, CA; ²Stanford University, Stanford, CA

ThP 470 **Quantitative Analysis of Bis(monoacylglycerol) phosphate and Phosphatidylglycerol Isomers by Shotgun lipidomics after One-step Methylation**; Miao Wang¹; Xianlin Han¹; ¹Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL

ThP 471 **A Miniaturized LC-MS/MS Platform for In-Depth Quantitative Profiling of Endocannabinoids and Related N-Acylethanolamines in Human Cerebrospinal Fluid**; Vasudev Kantae¹; Shinji Ogino¹; Marek Noga¹; Amy C Harms¹; Robin M. van Dongen²; Gerrit L. J. Onderwater²; Arn M. J. M. van den Maagdenberg²; Gisela M. Terwindt²; Mario van der Stelt¹; Michel D. Ferrari²; Thomas Hankemeier¹; ¹Leiden University, Leiden, Netherlands; ²Leiden University Medical Center, Leiden, Netherlands

ThP 472 **Accumulation of Oxygenated Phosphatidylethanolamines as Ferroptotic Death Signals Characterized by Oxidative Phospholipidomics**; Feng Qu¹; Yulia Y Tyurina¹; Jinming Zhao²; Gaowei Mao³; Vladimir A Tyurin¹; Tami Selvan Anthony-muthu³; Andrew A Amoscato¹; David R Emlet³; John A Kellum³; Sally E Wenzel²; Hülya Bayir³; Valerian E Kagan¹; ¹Departments



of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; ²Department of Medicine, University of Pittsburgh, Pittsburgh, PA; ³Department of Critical Care Medicine, University of Pittsburgh, Pittsburgh, PA

- ThP 473 **Global Profiling of FPP/GGPP-Protein Interactome in Liver via BSS-based Affinity Purification and Mass Spectrometry**; Jingzi Zhang^{1,2}; Lei Fang^{1,2}; Chaojun Li^{1,2}; ¹The Medical School of Nanjing University, Nanjing, China; ²Model Animal Research Centre of Nanjing University, Nanjing, China
- ThP 474 **Lipidomic Profiling of Targeted Oxylipins in Human Plasma with Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry**; Zhi-Xin Yuan¹; Christopher E Ramsden¹; ¹Lipid Mediators, Inflammation and Pain Unit, Laboratory of Clinical Investigation, National Institute on Aging, NIH., Bethesda, MD

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- ThP 475 **MALDI-MS/MS to Determine Sequencing Information of Novel Side Chain Liquid Crystalline Copolymers**; Savannah Snyder¹; Huiming Xiong²; Chrys Wesdemiotis³; ¹The University of Akron, Akron, Ohio; ²Shanghai Jiao Tong University, Shanghai, China; ³The University of Akron, Akron, OH
- ThP 476 **Nanoparticle Microarray for High-Throughput Microbiome Metabolomics Using Nanoparticle-Assisted Laser Desorption Ionization Mass Spectrometry**; Maria Emilia Dueñas¹; Rebecca Hansen¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- ThP 477 **Development of a Nanodiamond-based Multifunctional Platform for Bacteria Sensing, Identification, and Disinfection**; Chih-Che Wu; Department of Applied Chemistry, National Chi Nan University, Puli, Taiwan
- ThP 478 **AP-MALDI-Q-IMS-TOF MS as a Liquid Sample Mass Profiling Platform for Food Authenticity Tests**; Oliver John Hale¹; Michael Morris²; Rainer Cramer¹; ¹University of Reading, Reading, UK; ²Waters Corporation, Wilmslow, UK
- ThP 479 **Imaging Nanoparticle Drug Delivery Systems, their Cargo, and their Effect on Tissue Biochemistry by MALDI-MS**; Kristen Sikora¹; Laura Castellanos¹; Ying Jiang¹; Joseph Hardie¹; Vincent M Rotello¹; Richard W Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- ThP 480 **Investigation of the Binding Character of Potential Five Lipoxygenase Enzyme Inhibitors with On-Target Incubation**; Michael Ruehl¹; Benjamin Kuehn¹; Ute Bahr¹; Bettina Hofmann¹; Dieter Steinhilber¹; Michael Karas¹; ¹Goethe-University, Frankfurt am Main, Germany
- ThP 481 **Electron Transfer Ionization in MALDI-MS Using π -Extended Fluorenes as Matrices**; Juan S. Ramirez¹; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia
- ThP 482 **Cholesterol, Phospholipids and Glucose Detection in Vitreous Humor from Diabetic Human Donors**; Abigail Schnepf¹; M Cecilia Yappert¹; Douglas Borchman¹; ¹University of Louisville, Louisville, KY
- ThP 483 **MALDI MS Profiling of Serum Extracts to Identify Galactomannan Enzyme Immunoassay False Positivity via Immunoglobulin Products**; Matthew E. Openshaw¹; Tom K. Abban¹; Rebecca Gorton²; Simona Salivo¹; Ekta Patel¹; Emanuele Barborini³; Timothy D. McHugh⁴; Emmanuel Wey^{4,5}; ¹Shimadzu, Manchester, UK; ²Health Services Laboratories (HSL), London, UK; ³Tethis SpA, Milan, Italy; ⁴Centre for Clinical Microbiology, Division of Infection and Immunity, University College London, London, UK; ⁵Royal Free London NHS Trust Department of Clinical Microbiology, London, UK
- ThP 484 **Identification of Lipid Biomarkers of Human Inflammatory Bowel Disease Using Imaging Mass**

Spectrometry; Ekta Patel¹; Simona Salivo¹; Roberto Fernández²; Joan Bestard-Escalas³; Jone Garate²; Albert Maimó-Barceló³; Daniel H. López³; Sam Khorrami^{3,4}; Daniel Ginard^{3,4}; Gwendolyn Barceló-Coblijn³; José A. Fernández²; ¹Shimadzu, Manchester, UK; ²Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena, Spain; ³Research Unit, Hospital Universitari Son Espases, Institut d'Investigació Sanitària de Palma (IdISPa), Palma, Spain; ⁴Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain

- ThP 485 **Study of Oxidative Damage from Radiotherapy in HCT-116 Spheroids by MALDI Imaging**; Amaia Carrascal Minino¹; Fiona Henderson¹; Somrudee Deepaisarn¹; Kaye J Williams²; Adam McMahon¹; ¹Wolfson Molecular Imaging Centre, CRUK/EPSRC Imaging Centre of Cambridge & Manchester, The University of Manchester, Manchester, UK; ²Manchester Pharmacy School, University of Manchester, Manchester, UK
- ThP 486 **Analysis of Chlorophylls in Spinach (*Spinacia oleracea*) by Electron Transfer Ionization**; Juan S. Ramirez¹; Yoleisy Orduz¹; Julio R. Pinzón¹; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia
- ThP 487 **FTICR MALDI Analysis for Protein Footprinting and for Probing the Interaction of Warfarin with Vitamin K Epoxide Reductase**; Jerry Jiang; Washington University in St. Louis, St. Louis, MO
- ThP 488 **A Simplified Expedited Screening of Haemoglobinopathy and Pre-Diabetes in Whole Blood Using MALDI MS**; Tom K. Abban¹; Suzanne M. Docherty²; Jason K. Iles^{3,4}; Simona Salivo¹; Matthew E. Openshaw¹; Ray K. Iles³; ¹Shimadzu, Manchester, UK; ²Department of Haematology, Addenbrookes Hospital, Cambridge, UK; ³MAP Sciences Ltd, Bedford, UK; ⁴Department of Biotechnology and Chemical Engineering University of Cambridge, Cambridge, UK
- ThP 489 **Clinical Top-down Proteomics for Rapid Detection and Isotyping of Monoclonal Gammopathies**; Surendra Dasari¹; John R. Mills¹; Mindy C. Kohlhagen¹; David R. Barnidge¹; Angela Dispenzieri¹; David L. Murray¹; ¹Mayo Clinic, Rochester, MN
- ThP 490 **Sweet Beats! N-Glycan Changes in Allograft and Xenograft Heart Valves by MALDI Imaging Mass Spectrometry**; Peggi Angel¹; Anna Biemann²; Connor West¹; Kacey Talbot¹; Richard R Drake¹; Elizabeth Greene³; Lia H. Campbell³; Ulrich A Stock²; Kelvin Brockbank³; ¹Medical University of South Carolina, Charleston, SC; ²Royal Brompton and Harefield Foundation Trust, Imperial College, and Magdi Yacoub Institute, London, UK; ³Tissue Testing Technologies, LLC, Charleston, SC
- ThP 491 **Optimized MALDI-TOF Mass Spectrometry Workflow for Biomarker Discovery in Unfractionated Serum**; Maximilian Steers¹; Alex Nickel¹; Nicholas Dupuis¹; Gary Pestano¹; ¹Biodesix Inc, Boulder, CO

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- ThP 492 **Systemic Approaches for Understanding Regulatory Mechanisms Underlying Cancer Metabolism**; Iqbal Mahmud¹; Guimei Tian¹; Lisa Zhao¹; Timothy J. Garrett²; Daiqing Liao¹; ¹University of Florida, Gainesville, FL; ²University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL
- ThP 493 **Mapping of Greek Olive Oil Using FT-ICR Mass Spectrometry Flow Injection Analysis and Multivariate Data Analysis**; Matthias Witt¹; Theodora Nikou²; Aiko Barsch¹; Christopher J Thompson³; Maria Halabalaki²; ¹Bruker Daltonik GmbH, Bremen, Germany; ²University of Athens, Athens, Greece; ³Bruker Daltonic, Billerica, MA



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- ThP 494 **In-Source Ion Clustering of Bile Acids in ESI: Implications for Quantification, Instrument Operation and Non-Targeted Metabolomics Applications;** Patrick Brophy¹; Angela Doneanu²; Jay Johnson²; Corey D Broeckling¹; James Murphy²; Jessica E. Prenni¹; ¹Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; ²Waters Corp, Milford, MA
- ThP 495 **Discovery Single-cell Mass Spectrometry Profiles Metabolic Gradients in the 16-cell Vertebrate (Frog) Embryo;** Erika P Portero¹; Rosemary Masu Onjiko¹; Sally A Moody¹; Peter Nemes¹; ¹George Washington University, Washington, DC
- ThP 496 **Metabolic Signatures Reveal Exercise Training on Fatty Acid β -Oxidation in db/db Type 2 Diabetes Mellitus Mice;** Zongwei Cai¹; Li Xiang¹; ¹Hong Kong Baptist University, Kowloon Tong, Kowloon, China
- ThP 497 **A Novel Labeled Metabolomics Workflow applying Isotope Ratio Outlier Analysis (IROA) and SWATH® Acquisition for Unambiguous Compound Identification;** Baljit Ubhi¹; Felice de Jong²; Chris Beecher^{2,3}; ¹SCIEX, Redwood City, CA; ²IROA Technologies, Bolton, MA; ³University of Florida, Gainesville, FL
- ThP 498 **Untargeted Metabolomic Analysis of Porcine Serum and Oral Fluid with a MLV Porcine Reproductive and Respiratory Syndrome Virus (PRRSV) Vaccine;** Aislinn A Pomfret¹; David J Borts¹; Jeffery J Zimmerman¹; Yuly A Henao Diaz¹; Luis G Giménez-Lirola¹; Ting-Yu Cheng¹; ¹Iowa State University, Ames, IA
- ThP 499 **A Simplified, Integrated Solution for Untargeted Metabolomics;** Baljit Ubhi¹; Ranjan Perera²; Matthew Skaley¹; Timothy J. Garrett³; ¹SCIEX, Redwood City, CA; ²Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; ³University of Florida, Gainesville, FL
- ThP 500 **Metabolomic Analysis of Human Neural Stem Cells Using Nanoflow Liquid Chromatography-Tandem Mass Spectrometry;** Jingjing Deng¹; Guoan Zhang²; Thomas A. Neubert¹; ¹New York University Langone Medical Center, New York, NY; ²Weill Cornell Medicine, New York, NY
- ThP 501 **Metabolomics Approach to Evaluate Silver Nanoparticle Toxicity;** Samanthi I Wickramasekara¹; Suresh Narayanasamy¹; Steven Woolford¹; Eric Sussman¹; ¹US FDA, Silver Spring, MD
- ThP 502 **Single-cell Profiling of Dorsal-Ventral Metabolomic Differences in the Vertebrate (Frog) Embryo;** David Plotnick¹; Rosemary Masu Onjiko¹; Peter Nemes¹; ¹George Washington University, Washington, DC
- ThP 503 **Metabolomic Profiling in Human Mammary Epithelial Cells (HMEC) Exposed to 1,25(OH)2D3;** Renny S. Lan^{1,2}; Ping-Ching Hsu^{1,2}; Theodore M. Brasky²; Joseph P. McElroy²; Adana A. Llanos^{2,3}; Ken Riedl²; Steven J. Schwartz²; Peter G. Shields²; ¹University of Arkansas for Medical Sciences, Little Rock, AR; ²The Ohio State University, Columbus, OH; ³Rutgers University, New Brunswick, NJ
- ThP 504 **Comparative Metabolomics of Scab Resistant and Susceptible Pecans;** Zhentian Lei¹; David Huhman²; Daniel Wherritt³; Barbara Sumner¹; Santosh Kumar¹; Lloyd W. Sumner¹; ¹University of Missouri, Columbia, MO; ²The Samuel Roberts Noble Foundation, Ardmore, OK; ³University of Texas at San Antonio, San Antonio, TX
- ThP 505 **Derivatized Globally Optimized Targeted Mass Spectrometry (dGOT-MS) for Metabolomics Analysis of Carboxylic Acids;** Renke Zhang^{1,2}; Xinyu Zhang¹; Haiwei Gu¹; Ping Zhang^{1,3}; G. A. Nagana Gowda¹; Liladhar Paudel¹; Dan Du^{1,4}; Daniel Raftery¹; ¹Northwest Metabolomics Research Center, Department of Anesthesiology and Pain Medicine, University of Washington, Seattle, WA; ²China Agricultural University, Haidian, China; ³Southwest University, Beibei, China; ⁴West China-Washington Mitochondria and Metabolism Center, West China Hospital, Sichuan University, Chengdu, China
- ThP 506 **Comparison of High Resolution Quadrupole-Time-of-Flight and Orbitrap Mass Spectrometers for the Analysis of Small Molecules;** Marzieh Ramezani¹; Edgar A. Arriaga¹; ¹University of Minnesota, Minneapolis, Minnesota
- ThP 507 **Benefits of SWATH® Acquisition, a DIA Technique over Traditional Data Dependent Analysis for High Resolution Untargeted Metabolomics Applications;** Hector Gallart-Ayala¹; Zuzana Demianova²; Cyrus Papan³; Joerg Dojahn²; Baljit K. Ubhi⁴; ¹Sciex, Alcobendas, Spain; ²SCIEX, Darmstadt, Germany; ³SCIEX, Darmstadt, Germany; ⁴SCIEX, Redwood City, CA
- ThP 508 **Metabolic Profiling of Synthetic Cannabinoid 5F-ADB in Clinical Samples Using Non-Targeted SWATH Acquisition;** Michael Dunn¹; Margaret Knight¹; Clair Roper¹; Peter Blain¹; ¹Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK
- ThP 509 **High Throughput Metabolomics of Greenhouse Grown Maize Plants Reveals Response to Drought Treatments and Predicts Field Grain Yield;** Jan Hazebroek¹; April Agee Carroll²; Roland Welle³; Gerie van der Heijden¹; Teresa Harp¹; Chris Vlahakis¹; ¹DuPont Pioneer, Johnston, IA; ²Purdue, West Lafayette, IN; ³DuPont Pioneer, Eschbach, Germany
- ThP 510 **Metabolomic Profiling of Sweat Collected from Primary Lymphedema Patients Using Non-Occlusive Sample Collection and CIL LC-MS;** Kevin Hooton¹; Ian Soles²; Liang Li¹; ¹University of Alberta, Edmonton, AB, Canada; ²Salutaris Centre, Edmonton, AB, Canada
- ThP 511 **Achieving Rapid Multi-Omics Analysis in Under 48 Hours;** Alexander Aksenov¹; Robby Quinn¹; Jose Navas-Molina¹; Rob Knight¹; Pieter C. Dorrestein¹; ¹University of California San Diego, San Diego, CA
- ThP 512 **The Development of a LC-FAIMS-MS Metabolomics Workflow: A New Tool for Untargeted Metabolite Profiling to Diagnose Disease;** Lauren Brown¹; Kayleigh Arthur¹; Alasdair Edge¹; Aditya Malkar¹; Paul Nasca¹; ¹Owlstone Medical Ltd., Cambridge, UK
- ThP 513 **Untargeted Metabolic Profiling of the Media of *Plasmodium falciparum* Isolates Grown to Different Levels of Parasitemia;** Patricia Gonzales Hurtado¹; Benjamin Orsburn²; Michal Fried¹; ¹Laboratory of Malaria Immunology and Vaccinology, NIAID, Rockville, Maryland; ²Thermo Fisher Scientific, West Palm Beach, FL
- ThP 514 **Global Metabolomics Profile through the Blood-Brain Barrier of the Neurovascular Unit (NVU);** Simona Gabriela Codreanu^{1,2}; Stacy D. Sherrod^{1,2}; Jacquelyn A. Brown¹; Diana M. Neely³; BethAnn McLaughlin³; Aaron B. Bowman³; John P. Wikswol¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN; ²Center for Innovative Technology, Vanderbilt University, Nashville, TN; ³Vanderbilt University Medical Center, Nashville, TN

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- ThP 515 **Interconversion of Protonated Imidazolidinone Ions; Isomers of [b4]⁺ Derived from Protonated Tetraglycine;** Brian Lam¹; Justin Kai-Chi Lau^{1,2}; Cheuk-Kuen Lai^{1,2}; K.W. Michael Siu^{1,2}; Alan C. Hopkinson¹; ¹York University, Toronto, ON, Canada; ²University of Windsor, Windsor, ON, Canada
- ThP 516 **Formation of Protonated a and b Ions from Lanthanide-Peptide Complexes;** Yating Wang¹; Justin Kai-Chi Lau¹; Cheuk-Kuen Lai^{1,2}; Brian Lam¹; K.W. Michael Siu^{1,2}; Alan C. Hopkinson¹; ¹York University, Toronto, ON, Canada; ²University of Windsor, Windsor, ON, Canada
- ThP 517 **Fragmentation Mechanism of Proline Containing Dipeptide;** Sabyasachy Mistry; ¹Purdue University, West Lafayette, IN



- ThP 518 **Fragmentation of Deprotonated Glycine and Alanine, their Di-, Tri-Peptides and Corresponding Amides Investigated by Collision-Induced Dissociation and Molecular Orbital Calculations;** Can Cui¹; Ashley S. McNeill²; David A. Dixon²; Carolyn J. Cassady²; ¹The University of Alabama, Tuscaloosa, AL; ²The University of Alabama, Tuscaloosa, AL

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- ThP 519 **Evolution of a Mass Spectrometry-Grade PTM Directed Protease for Large Scale Post-Translational Modification Analyses;** Duc Tran^{1,2}; Valerie J. Cavett²; Vuong Q. Dang²; Hector L. Torres²; Brian M. Paegel²; ¹Ho Chi Minh City International University, Ho Chi Minh City, Vietnam; ²The Scripps Research Institute, Jupiter, FL
- ThP 520 **Rapid and Accurate Global PTM Discovery (G-PTM-D) Using Defined Mass Windows;** Stefan K. Solntsev¹; Michael R. Shortreed¹; Brian L. Frey¹; Robert J. Millikin¹; Anthony J. Cesnik¹; Lloyd M. Smith^{1,2}; ¹University of Wisconsin-Madison, Madison, WI; ²Genome Center of Wisconsin, Madison, WI
- ThP 521 **Accurate Phosphorylation Site Localization Using Phospho-containing Site-determining Product Ions;** Zhixin Tian¹; Kaijie Xiao¹; ¹School of Chemical Science and Engineering, Tongji University, Shanghai, China
- ThP 522 **Nontargeted Characterization of D-Amino Acid-Containing Neuropeptides;** Itamar Livnat¹; Hua-Chia Tai²; Elena V. Romanova²; James W. Checco²; Jonathan V. Sweedler²; ¹University of Illinois at Urbana-Champaign, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- ThP 523 **Characterization of L/D-Peptide Isomerase Activity in *Aplysia californica*;** Hua-Chia Tai¹; Peter M. Yau²; Jonathan V. Sweedler²; ¹University of Illinois at Urbana-Champaign, Urbana, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL
- ThP 524 **Defining Mechanisms of Licorice Chemoprevention: Identification of Active Sites on Keap1 and Bach1 Regulating the Antioxidant Response Element;** Amanda Lee¹; Lingyi Huang¹; Richard B. van Breemen¹; ¹University of Illinois at Chicago College of Pharmacy, Chicago, IL
- ThP 525 **Characterization of tau Post-Translational Modifications in a Novel Cellular Model of tau Aggregation;** Nathan G. Hatcher¹; Mali L. Cosden¹; Daniel S. Spellman¹; John M. Majercak¹; Joel B. Schachter¹; ¹Merck Research Laboratories, West Point, PA
- ThP 526 **The Highly Ubiquitinated Protein Cargo of Exosomes Shed by Myeloid-Derived Suppressor Cells;** Sitara Chauhan¹; Katherine Adams¹; Virginia Clements²; Yan Wang¹; Nathan J. Edwards³; Suzanne Ostrand-Rosenberg²; Catherine Fenselau¹; ¹University of Maryland, College Park, MD; ²University of Maryland Baltimore County, Baltimore, MD; ³Georgetown University Medical Center, Washington, DC, DC
- ThP 527 **Large Scale Discovery of Post-Translational Modifications Conserved across Microbial Species;** Seunghun Na¹; Nuno Bandeira¹; ¹University of California, San Diego, La Jolla, CA
- ThP 528 **Subcritical Water Processing of Proteins: Amino acid side-chain modifications;** Thomas Powell¹; Helen J. Cooper¹; Steve Bowra²; ¹University of Birmingham, Birmingham, UK; ²Phytatec (UK) Ltd, Plas Gogerddan, UK
- ThP 529 **Retention Time Prediction for Glycopeptides in Reversed phase Chromatography;** Evelyn Ang¹; Vic Spicer¹; Helene Perreault¹; Oleg Krokhin¹; ¹University of Manitoba, Winnipeg, MB
- ThP 530 **Retention Time Prediction for Peptides Containing Deamidated Asn Residues in Reversed-Phase Chromatography;** Haley Neustaeter¹; Victor Spicer¹; Oleg Krokhin¹; ¹University of Manitoba, Winnipeg, MB
- ThP 531 **Controlling the False Amino-acid Rate (FAR) in De Novo Peptide Sequencing;** Hao Yang¹; Hao Chi¹; Wen-Feng Zeng¹; Wen-Jing Zhou¹; Chao Liu¹; Si-Min He¹; ¹Key Lab of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Beijing, China
- ThP 532 **Simple, Rapid Determination of Isobaric Amino Acids by Chemical Derivatization;** Stephen Ayrton¹; Ryan M. Bain²; Christopher J. Pulliam²; Tawnya Flick³; R. Graham Cooks²; ¹West Lafayette, IN; ²Purdue, West Lafayette, IN; ³Amgen, Thousand Oaks, CA
- ThP 533 **Antibody-based Target Identification of Covalent Kinase Inhibitors and Potential Targets of Phenyl Vinyl Sulfone by Mass Spectrometry;** Chi-Chi Chou¹; Cheng-Han Yu²; Geen-Dong Chang²; Kay-Hooi Khoo^{2,3}; ¹Academia Sinica, Taipei; ²National Taiwan University, Taipei, Taiwan; ³Academia Sinica, Taipei, Taiwan
- ThP 534 **Precipitation of HPG-ALD Polymer Using Organic Solvents Improves Peptide Identification in TAILS Terminomics;** Nestor Solis¹; Jennifer Mark¹; Anilkumar Parambath¹; Jayachandran Kizhakkedathu¹; Christopher M. Overall¹; ¹University of British Columbia, Vancouver, BC, Canada
- ThP 535 **Discovery and Identification of O-Glycosylated Signaling Peptides from Mouse and Human Pancreatic Islets Enabled by EThcD Mass Spectrometry;** Qing Yu¹; Alejandra Canales²; Matthew Glover²; Rahul Das²; Xudong Shi²; Yang Liu²; Mark P. Keller²; Alan D. Attie²; Lingjun Li²; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin-Madison, Madison, WI
- ThP 536 **Systematic Comparison of Reduction and Alkylation Reagents reveals Side Chain Loss of Methionine due to Iodine Containing Alkylation Reagents;** Torsten Müller¹; Dominic Winter¹; ¹IBMB Bonn, Bonn
- ThP 537 **Developing an Analytical Framework for Sulfoliproteomics: Sulfolipopeptide Enrichment and Positive Mode Mass Spectrometric Analysis;** Hye Kyong Kweon¹; Brian L. Tang¹; Phillip J. McClory¹; Philip C. Andrews¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI
- ThP 538 **Data-Independent Infrared Multi-Photon Dissociation for the Targeted Discovery of Cysteine Sulfonic Acid;** Nicholas B. Borotto¹; Phillip J. McClory²; Brent R. Martin²; Kristina Hakansson²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, Michigan
- ThP 539 **HILIC LC/MS Analytical Approach for Identification of Protein Deamidation and Isomerization Modifications;** Barry Boyes^{1,2}; Majors Badgett²; Ron Orlando²; ¹Advanced Materials Technology Inc., Wilmington, DE; ²Complex Carbohydrate Research Center, University of Georgia, Athens, GA
- ThP 540 **Evaluation of Methods for Selective Isolation of Cysteine-Containing Peptides in Redox-Proteomics;** Muhammad Tahir¹; Honggang Huang¹; Martin R. Larsen¹; ¹Univ. Southern Denmark, Odense
- ThP 541 **Mass Spectrometry Analysis of Sulfonation Cysteines in Peroxiredoxin 1;** Changgong Wu¹; ¹Center for Advanced Proteomics Research and the Department of Microbiology, Biochemistry and Molecular Genetics, Rutgers University, Newark, NJ
- ThP 542 **Optimization of SimSpectraST Search Conditions for Phosphoproteomics;** Tomoya Tsubosaka¹; Ayano Takai¹; Satoko Akahori¹; Seiya Kawahara¹; Veronika Suni²; Susumu Y. Imanishi¹; ¹Meijo University, Nagoya, Aichi; ²University of Turku, Turku, Finland



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- ThP 543 **Multiplex Quantitation of Crustacean Neuropeptides after Hypoxia Exposure Using Custom 4-plex Dimethylated Leucine (DiLeu) Isobaric Tags;** Chris Sauer¹; Amanda Buchberger¹; Kellen DeLaney¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 544 **Multifaceted Quantitation and Imaging of Changes in Crustacean Neuropeptidome Resulting from Food Intake;** Kellen DeLaney¹; Lingjun Li^{1,2}; ¹University of Wisconsin - Madison Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison School of Pharmacy, Madison, WI
- ThP 545 **Induced Expression of Bioactive Peptides in *Solanum lycopersicum* under Salt Stress Conditions;** Tessa E. Bartges¹; Christine L. Kirkpatrick¹; Nazia Kanwal²; Amer Jamil²; Leslie M. Hicks¹; ¹Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Department of Biochemistry and Molecular Biology, University of Agriculture Faisalabad, Faisalabad, Pakistan
- ThP 546 **Functional Discovery of Neuropeptides in Blue Crab, *Callinectes sapidus*, in Response to Ocean Acidification;** Yang Liu¹; Amanda Buchberger¹; Kellen DeLaney¹; Lingjun Li^{1,2}; ¹University of Wisconsin - Madison Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison School of Pharmacy, Madison, WI
- ThP 547 **Profiling Peptidomic Changes in Major Brain Regions in Response to Cocaine Intoxication and Withdrawal;** Fengfei Ma¹; Pingli Wei²; Jingxin Wang³; Vaishali Bakshi³; Brian Baldo³; Lingjun Li^{1,2}; ¹University of Wisconsin-Madison School of Pharmacy, Madison, WI; ²University of Wisconsin - Madison Department of Chemistry, Madison, WI; ³University of Wisconsin-Madison, Madison, WI
- ThP 548 **Differential Quantification of Ageing and Dehydration Effects on Peptide Secretion in the Pituitary by Automated MALDI-TOF MS;** Elena Romanova¹; Michael P. Greenwood²; Mingkwan Greenwood²; David Murphy²; Jonathan V. Sweedler³; ¹University of Illinois at Urbana-Champaign, Urbana, IL; ²University of Bristol, Bristol, UK; ³University of Illinois at Urbana Champaign, Urbana, IL
- ThP 549 **Multifaceted Mass Spectrometric Analyses of Feeding-related Metabolomic and Peptidomic Changes in the Rock Crab, *Cancer irroratus*;** Qinjingwen Cao¹; Qing Yu²; Bingming Chen²; Chuanzi OuYang¹; Fengfei Ma²; Lingjun Li^{1,2}; ¹Department of chemistry, University of Wisconsin Madison, Madison, WI; ²School of pharmacy, University of Wisconsin Madison, Madison, WI
- ThP 550 **Peptidogenomic Capture of Microprotein Virulence Factors in Community-Associated *Staphylococcus aureus*;** Jacob Wozniak¹; John Lapek¹; Julieta Aguilar¹; Dominic McGrosso¹; David Gonzalez¹; Michael Does²; Ross Corriden¹; Anvesh Marchela¹; JoAnn Trejo¹; Eri Nakatani-Webster³; Abhinav Nath³; Brian Werth³; ¹UCSD, La Jolla, CA; ²Hofstra Northwell School of Medicine, Hempstead, NY; ³University of Washington, Seattle, WA
- ThP 551 **Top-down and Bottom-up Proteomics for the Identification of Crustacean Neuropeptides and Precursor-Related Peptides Predicted by Transcriptomics;** Cindy Rivera¹; Julia M. Michels¹; Caroline Q. Corban¹; Patsy S. Dickinson¹; Andrew E. Christie²; Elizabeth A. Stemmler¹; ¹Bowdoin College, Brunswick, ME; ²University of Hawaii at Manoa, Honolulu, Hawaii

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Notre Dame, IN; ²Michigan State University, Lansing, MI; ³University of Wisconsin-Madison, Madison, WI

- ThP 553 **Time-Resolved Quantitative Analysis of Cellular Signaling and Epigenetic Mechanisms During Epithelial-Mesenchymal Transition;** Congcong Lu¹; Simone Sidoli¹; Zuofei Yuan¹; Benjamin A. Garcia¹; ¹University of Pennsylvania, Philadelphia, PA
- ThP 554 **Accumulated Ion Monitoring (AIM) Enables Enrichment-Free Quantitation of Rare and Phosphorylated Peptides from Micrograms and Thousands of Human Cells;** Paolo Cifani¹; Alex Kentsis^{1,2}; ¹Molecular Pharmacology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY; ²Department of Pediatrics, Weill Medical College of Cornell University and Memorial Sloan Kettering Cancer Center, New York, NY
- ThP 555 **Dephosphorylation of AMA1 Cytosolic Tail during *Toxoplasma gondii* Invasion;** Shruthi Krishnamurthy¹; Bin Deng¹; Roxana del Rio¹; Kerry R. Buchholz²; Moritz Treec²; Siniša Urban³; John Boothroyd²; Ying Wai Lam¹; Gary E. Ward¹; ¹University of Vermont, Burlington, VT; ²Stanford School of Medicine, Stanford, CA; ³Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 556 **A Phosphoproteomic Approach to Investigate Mechanical Sensing in *Xenopus laevis* Embryos;** Yutaka Hashimoto^{1,2}; Noriyuki Kinoshita²; Todd M. Greco¹; Pierre Jean Beltran¹; Joel Federspiel¹; Naoto Ueno²; Ileana M. Cristea¹; ¹Princeton University, Princeton, NJ; ²National Institute for Basic Biology, Okazaki, Japan
- ThP 557 **Identification of Potential Mitotic CK2 Substrates and Interactors by Quantitative Phosphoproteomics;** Scott Rusin¹; Arminja N Kettenbach^{1,2}; ¹Dartmouth College, Hanover, NH; ²Norris Cotton Cancer Center, Lebanon, NH
- ThP 558 **Nano LC-MS Based Phosphoproteomic Approach for Evaluating Signaling Properties of Insulin Receptor Agonists;** Zhongping Liao¹; Jason X. Tang²; ¹Eli Lilly and Company, Indianapolis, IN; ²Eli Lilly and Company, Indianapolis, IN
- ThP 559 **Quantitative Chemical Phosphoproteomics Identifies PCTAIRE-1 (Cdk16) as a Novel Wee1 Substrate;** Andrew Grasseti¹; Rufus Hards²; Scott A Gerber²; ¹Lebanon, NH; ²Dartmouth College, Hanover, NH
- ThP 560 **Kinase Activity Profiling by Motif-Targeting Phosphoproteome Analysis;** Chia-Feng Tsai¹; Masaki Wakabayashi¹; Naoyuki Sugiyama¹; Yasushi Ishihama¹; ¹Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto City, Japan
- ThP 561 **Benchmarking LFQ, SILAC and MS2/MS3-based TMT Quantification Strategies for Phosphoproteomics;** Alexander Hogrebe¹; Louise von Stechow¹; Dorte B. Bekker-Jensen¹; Brian T. Weinert¹; Christian D. Kelstrup¹; Jesper V. Olsen¹; ¹The Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- ThP 562 **Multiplexing Meets Automation: TMT-Labeling in PRM Assays Increases Sample Throughput and Allows for Precise Relative Quantification;** Malvina Papanastasiou¹; Alvaro Sebastian Vaca Jacome¹; Adam Officer¹; Katherine DeRuff¹; Steven A. Carr¹; Jacob D. Jaffe¹; ¹Broad Institute of MIT and Harvard, Cambridge, Massachusetts
- ThP 563 **Identification of physiological kinase substrates from cell extracts by differential phosphorylation using reverse in-gel kinase assay and nano-LC tandem MS;** Weiliang Huang¹; Xiang Li²; Keqi Tang³; Maureen A. Kane¹; Charles J. Bieberich²; ¹University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; ²University of Maryland Baltimore County, Department of Biological Sciences, Baltimore, MD; ³Pacific Northwest National Laboratory, Biological Sciences Division, Richland, WA



- ThP 564 **Establishing the Basal Global Phosphorylation Stoichiometry of a Human Colorectal Carcinoma Cell Line Using TMT-Based Multiplexed Proteomics;** Matthew Y. Lim¹; Joao A. Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA
- ThP 565 **Quantitative Phosphoproteomic Analysis of Circadian Clock-Associated Kinases in *Arabidopsis thaliana*;** Shin-Cheng Tzeng¹; Margret Wilson¹; Matthew Meyer¹; Xiaoyue Jiang²; Jae Choi³; John Bulter²; Dmitri Nisnow¹; Bradley Evans¹; ¹Donald Danforth Plant Science Center, St. Louis, MO; ²Thermo Fisher Scientific, San Jose, California; ³Thermo Fisher Scientific, Rockford, IL
- ThP 566 **Quantitative Phosphoproteomics Unveils Novel phosphorylation Events in Transformed Human Bronchial Epithelial Cell Induced by Arsenic;** Yue Qi¹; Lingzhi Li¹; Michael Caruso¹; Xiangmin Zhang¹; Fei Chen¹; Zhengping Yi¹; ¹Wayne State University, Detroit, Michigan
- ThP 567 **Going Deep: A Comprehensive Analysis of Tissue-Specific Protein Phosphorylation and Expression;** Katie J. Clowers¹; Mark P. Jedrychowski¹; Edward L. Huttlin¹; John Szpyt¹; Joao A. Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA
- ThP 568 **The Phosphoproteome as a Phenotype: Towards a high throughput Platform for Phosphoproteomics;** Matthew Foley^{1,2}; Michael J. Ford²; Richard C. Jones²; Ravi Amunugama²; David L. Allen²; ¹University of Michigan, Ann Arbor, Michigan; ²MS Bioworks, Ann Arbor, MI
- ThP 569 **High-Resolution Phosphoproteomic Identification of Zika Virus-Initiated Events in Host Cells;** Ronik Khachatourian¹; Whitaker Cohn²; Austin Quach²; James Vu¹; Natalie Liu¹; Nu Lu¹; Travis Moller²; Piotr Ruchala²; Vaithilingaraja Arumugaswami³; Samuel French¹; Julian Whitelegge²; ¹Department of Pathology and Laboratory Medicine, David Geffen School of Medicine at University of California, Los Angeles, CA; ²Pasarow Mass Spectrometry Laboratory and Neuropsychiatric Institute—Semel Institute for Neuroscience & Human Behavior, David Geffen School of Medicine at UCLA, Los Angeles, California; ³Department of Surgery, The Board of Governors Regenerative Medicine Institute at Cedars-Sinai Medical Center, Los Angeles, CA
- PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION 570 - 605**
- ThP 570 **Prediction of Deamidation Rates of Proteins to Assess their Long-Term Stability Using Hydrogen Exchange Mass Spectrometry (HX-MS);** Chamalee L.D. Gamage¹; David D. Weis^{1,2}; ¹Department of Chemistry, University of Kansas, Lawrence, KS; ²Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS
- ThP 571 **Site-Specific Characterization of PEGylated Insulin Isomers by Using Combined Liquid Chromatography and Ion Mobility Mass Spectrometry;** Selim Gerislioglu¹; Scott Adams¹; Chrys Wesdemiotis¹; ¹The University of Akron, Akron, OH
- ThP 572 **Applications of Native Mass Spectrometry (MS) for Biotherapeutics Characterization and Associated Challenges;** Olga Friesse¹; Thomas W. Powers¹; Jacquelynn Smith¹; Paul Brown¹; Andrew Dawdy¹; Jason C. Rouse²; ¹Pfizer, Inc., St. Louis, MO; ²Pfizer, Inc., Andover, MA
- ThP 573 **Discovery, Characterization, and Remediation of an Fc-extension in Proteins Expressed in CHO Cells;** Stone D.-H. Shi¹; Christopher S. Spahr¹; Mark E. Daris¹; Kevin C. Graham¹; Brian D. Soriano¹; Jennitte L. Stevens¹; ¹Amgen, Thousand Oaks, CA
- ThP 574 **Orthogonal Mass Spectrometry-Based Footprinting Strategies Characterize the Epitope and a Structural Rearrangement of Interleukin-6 Receptor Subunit Alpha upon Adnectin Binding;** Ke Sherry Li¹; Guodong Chen²; Jingjie Mo²; Richard Y.-C. Huang²; Ekaterina Deyanova²; Brett Beno²; Steve O'neil²; Adrienne A. Tymiak²; Michael L. Gross³; ¹Washington University, St. Louis, MO; ²Bristol-Myers Squibb, Princeton, NJ; ³Washington University, St. Louis, MO
- ThP 575 **Mapping of Complex Disulfide Patterns with Closely-Spaced Cysteines by In-Source Reduction and Data-Dependent Mass Spectrometry;** Christian Cramer^{1,2}; Christian D. Kelstrup²; Jesper V. Olsen²; Kim F. Haselmann¹; Peter Kresten Nielsen¹; ¹Novo Nordisk A/S, Maaloev, DK; ²CPR - Center for Protein Research, Copenhagen, Denmark
- ThP 576 **Development of a Fast Proteinase K Digestion Protocol for Characterization of Fluorescein Isothiocyanate Labeled Recombinant Human Insulin;** Fanyu Meng¹; Ross Yang¹; Weijuan Tang¹; Li-Kang Zhang¹; Bing Mao¹; ¹Merck & Co., Inc, Rahway, NJ
- ThP 577 **Automated Determination of Induced Monoclonal Antibody Disulfide Bond Shuffling Using Multiple Enzyme Digestions;** Christopher A. Bolcato¹; Katy Ryan¹; Heather Anderson¹; Matthew J. Powell¹; K. Ilker Sen²; St. John Skilton²; Eric Carlson³; Matthew D. Maust¹; ¹Protea Biosciences, Morgantown, WV; ²Protein Metrics, San Carlos, CA; ³Protein Metrics Inc., San Carlos, CA
- ThP 578 **Characterization of a Novel Modification of a CHO Produced mAb: Evidence for the Presence of Tyrosine Sulfation;** Jia Zhao; Merck, Kenilworth, NJ
- ThP 579 **Optimizing Biotherapeutics Size-based Characterization by Native Mass Spectrometry;** Leah (Hanliu) Wang¹; Thomas W. Powers¹; Ying Zhang²; Cliff Enrican²; Jacquelynn Smith¹; Andrew W. Dawdy¹; Yin Luo²; Jason C. Rouse²; OLGA FRIESE¹; ¹Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; ²Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MA
- ThP 580 **Subtle Structural Changes to Antibody Therapeutics Detected Using Diethylpyrocarbonate Labeling and Mass Spectrometry;** Patanachai (Kong) Limpikirati¹; John E. Hale²; Eric M. Graban²; Robert C. Vaughan³; Richard W. Vachet¹; ¹Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; ²QuarryBio, Bloomington, IN; ³Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN
- ThP 581 **Study of Stressed Monoclonal Antibody (mAb) Pharmaceuticals by Using Deep-UV Resonance Raman (DUVRR) Spectroscopy and MALDI-TOF Mass Spectrometry;** Chen Qiu¹; Jamie Mans¹; Sergey Arzhantsev¹; ¹US FDA, St. Louis, MO
- ThP 582 **Tyrosine to Phenylalanine Sequence Variants Observed During Cell Line Development for Manufacture of a Monoclonal Antibody;** Thomas Slaney¹; Mina Chaudhry¹; Hangtian Song¹; Wei Wu¹; Li Tao¹; Tapan Das¹; ¹Bristol-Myers Squibb, Hopewell, NJ - New Jersey
- ThP 583 **Dialysis-Coupled Hydrogen/Deuterium Exchange Mass Spectrometry Allows Conformational Analysis of Therapeutic Monoclonal Antibodies at Extreme Concentrations;** Zeinab Nazari^{1,2}; Damian Houde³; Marco van de Weert¹; George Bou-Assaf²; Andrew Weiskopf²; Kasper Dyrberg Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Department of Protein Pharmaceutical Development, Biogen, Cambridge, MA; ³Codiak BioSciences, Cambridge, MA
- ThP 584 **Data Independent Top-Down Characterization of Proteins for Biotherapeutic Applications;** Lindsay Morrison¹; Brad Williams¹; ¹Waters Corporation, Beverly, MA
- ThP 585 **Detection and Characterization of N- and O-Glycosylation: Streamlined Methods for Intact Mass Analysis and Bottom-Up Proteomics;** Paula Magnelli¹; Colleen McClung¹; Cristian Ruse¹; Ellen Guthrie¹; Stephen Shi¹; ¹New England Biolabs, Ipswich, MA
- ThP 586 **Impact of Tryptophan Oxidation in Complementarity-Determining Regions on Structure-Function Characterized by Hydrogen Exchange Mass Spectrometry and Surface Plasmon Resonance;** Tyler



THURSDAY POSTERS

- ThP 587 **Hageman^{1,2}; Hui Wei²; Patrick Kuehne²; Jinmei Fu²; Richard Ludwig²; Li Tao²; Tapan Das²; ¹University of Kansas, Lawrence, KS; ²Bristol-Myers Squibb, Pennington, NJ**
Direct Mass Spectrometric Characterization of Disulfide Linkages; Xiaoyan Guan¹; Le Zhang¹; Jette Wypych¹; ¹Amgen Inc., Thousand Oaks, CA
- ThP 588 **Toward Chemical Footprinting at Residue Resolution: FPOP Data Analysis of IL23 - Antibody Binding; Jing Li¹; Ke Li¹; Michael L. Gross¹; Ekaterina Deyanova²; Richard Huang²; Yun Wang²; Robert Langish²; Adrienne A. Tymiak²; Guodong Chen²; Kadir Ilker Sen³; Eric Carlson³; Christopher Becker³; ¹Washington University, St Louis, MO; ²Bristol-Myers Squibb, Princeton, NJ; ³Protein Metrics Inc., San Carlos, CA**
- ThP 589 **Capillary Electrophoresis - Mass Spectrometry (IP-CE-MS) Analysis of Protein Therapeutics for Identification of *in vivo* Catabolites; Mei Han¹; Josh T. Pearson¹; Yunan Wang¹; Dan A. Rock¹; Brooke M. Rock¹; ¹Amgen, South San Francisco, CA**
- ThP 590 **Sample Preparation Method for Accurate Analysis of Non-Enzymatic PTMs in Biotherapeutic Proteins with Peptide Mapping; Sergei Saveliev¹; Chris Hosfield¹; Michael Rosenblatt¹; Marjeta Urh¹; ¹Promega Corporation, Madison, WI**
- ThP 591 **Protein Disulfide Bond Characterization with DMS and ECD; J.C. Yves Leblanc¹; Brendon Seale^{1,2}; Lyle Burton¹; Takashi Baba¹; ¹SCIEX, Concord, ON, Canada, ON, Canada; ²University of Toronto, Toronto, ON, Canada**
- ThP 592 **Improvement of Glycosylation Profile to Increase Similarity of Adalimumab Biosimilar to the Innovator with High-Resolution Mass Spectrometry; Ahmet Emin Atik¹; Zeynep Yildirim Keles¹; Yigit Erdemgil¹; Deniz Baycin Hizal¹; Ozge Can²; R. Serdar Alpan¹; ¹Turgut Ilaclari Biotechnology Group, Istanbul, Turkey; ²Department of Medical Engineering, Acibadem University, Istanbul, Turkey**
- ThP 593 **Characterizing Monoclonal Antibody (mAb) Epitopes and Paratopes Using Structural Mass Spectrometry; Janna Kiselar^{1,2}; John Schenkel³; Mark Chance^{2,4}; ¹Case Western Reserve University, Cleveland, OH; ²Department of Nutrition, Case Western Reserve University, Cleveland, OH; ³NeoProtoemics, Inc., Cleveland, OH; ⁴Case Western Reserve University, Cleveland, OH**
- ThP 594 **Systematic Analysis of the Truncations and Modifications of Bovine Pulmonary Surfactant Proteins B and C in Natural Alternative Medicine; Lian Shu¹; Jifeng Wang¹; Zhengsheng Xie¹; Lili Niu¹; Xiang Ding¹; Xiaojing Guo¹; Tanxi Cai¹; Fuquan Yang²; ¹Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; ²Institute of Biophysics, CAS, Beijing, Beijing**
- ThP 595 **An Improved Workflow for Sequence Confirmation and PTM Identification of Monoclonal Antibodies Using Middle-Down ETD and CID Fragmentation; Weibin Chen¹; Henry Shion¹; Nilini Ranbaduge¹; Francesco Lanucara²; Emmy Hoyes²; Jeff Brown²; Jonathan P Williams²; James Langridge²; ¹Waters Corp, Milford, MA; ²Waters Corp., Wilmslow, UK**
- ThP 596 **A Multi-level Quantitative Estimation of mAb Clipping; Harsha Gunawardena¹; Eric Beil¹; Andy Mahan¹; Jeff Brelsford¹; Hirsh Nanda¹; ¹Janssen R&D of Johnson & Johnson, Greater Philadelphia, PA**
- ThP 597 **Comprehensive Characterization of the NIST mAb Reference Standard Using an IMS QToF Mass Spectrometer; Nilini Ranbaduge¹; Jing Fang²; William Alley²; Henry Shion²; Ying Qing Yu²; ¹Waters Corporation, Milford, Massachusetts; ²Waters Corp, Milford, MA**
- ThP 598 **Native Ion Exchange Chromatography Orbitrap Mass Spectrometry Allows Surface Charge Discrimination and Online Detection of Intact Proteins for Deep Characterization; Aaron O. Bailey¹; Guanghui Han²; Wendy Sandoval²; Jonathan L. Josephs¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Genentech, Inc, South San Francisco, CA**
- ThP 599 **A General Optimized Protocol for Sequence and Glycoforms Characterization of Monoclonal Antibodies; Modupeola A Sowole¹; Lin He²; Baozhen Shan²; Gilles A. Lajoie³; ¹University of Western Ontario, London, ON, Canada; ²Bioinformatics Solutions Inc, Waterloo, ON, Canada; ³University of Western Ontario, London, ON, Canada**
- ThP 600 **Development of LC-MS Platform Methods for IgG Analysis Using Q-Exactive Plus; Alisa Marie VanGrunsven¹; Emilie Aude Viglino¹; ¹CMC Biologics, Bothell, Washington**
- ThP 601 **High Efficiency Wide Pore Superficially Porous Particles for LC/MS of Larger Proteins; Stephanie A. Schuster¹; Brian M. Wagner¹; Benjamin P. Libert¹; William L. Miles¹; Barry E. Boyes^{1,2}; ¹Advanced Materials Technology, Inc., Wilmington, DE; ²Complex Carbohydrate Research Center, University of Georgia, Athens, GA**
- ThP 602 **Automated Intact Mass Analysis for the Characterization of Antibodies; Maurizio Bronzetti¹; Joe Shambaugh¹; David Bush¹; Stefano Gotta²; Cassandra Wigmore²; Arnd Brandenburg²; ¹Genedata Inc, Lexington, MA; ²Genedata AG, Basel, Switzerland**
- ThP 603 **Higher Order Structure of Intact Proteins by Capillary Electrophoresis Native Ion Mobility Mass Spectrometry; Caroline S. Chu¹; Pat D. Perkins²; Andy Gieschen³; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Agilent Technologies Inc., Santa Clara, CA; ³Agilent Technologies Inc., La Jolla, CA**
- ThP 604 **Simple and Quick MS Analysis of Chemically Synthesized Glycopeptides: Hydrogen/Deuterium Exchange (HDX)/MS for Verifying Racemization; Izumi Sakamoto¹; Kenji Hirose²; ¹AcroScale Inc., Sendai, Japan; ²Nihon Waters K.K., Osaka, Japan**
- ThP 605 **Pulsed HDX-MS Probes Protein Aggregate Intermediates – Preliminary Study of GCSF Aggregation; Jun Zhang¹; Michael J. Treuheit¹; ¹Amgen, Inc, Thousand Oaks, CA**

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- ThP 606 **Characterization of Protein Recognition Motifs within Heparin Chains: Online Size Exclusion Chromatography-Mass Spectrometry Based Solution Phase Footprinting; Chendi Niu¹; Yunlong Zhao¹; Igor A. Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA**
- ThP 607 **Studying Protein-Protein Complexes by Gas-Phase hydrogen/Deuterium Exchange Mass Spectrometry (Gas-Phase HDX-MS); Ulrik Hvid Mistarz¹; Shane A Chandler²; Justin L P Benesch²; Kasper D Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²Department of Chemistry, University of Oxford, Oxford, UK**
- ThP 608 **Gas Phase Activation Energies of Protein-Protein Interactions Determined by Electrospray Mass Spectrometry; Yelena Yefremova¹; Teresa F.I. Melder¹; Bright D. Danquah¹; Kwabena F.M. Opuni¹; Cornelia Koy¹; Knut Koelbel²; Frank Sobott²; Harald Illges³; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²University of Antwerp, Antwerp, Belgium; ³University of Applied Sciences Bonn-Rhein-Sieg, Bonn, Germany**
- ThP 609 **Engineering Nanodiscs for Membrane Protein Native Mass Spectrometry; Michael Thomas Marty; University of Arizona, Tucson, AZ**
- ThP 610 **Binding Affinity and Kinetics of Transient Protein-Protein Interactions by SEC/MS Measurements; Honglin Yao¹; Muneeruddin Khaja¹; Andrei N. Lipatnikov²; Cedric E. Bobst¹; Igor A. Kaltashov¹; ¹University of Massachusetts**



- Amherst, Amherst, MA; ²Chalmers University of Technology, Gothenburg, Sweden
- ThP 611 **Quantifying Non-Covalent Complexes of Insulin with Ca(II), Mg(II), Na(I) and K(I) Electrolyte Ions by Using ESI-MS Method**; Mustafa Gulfer¹; Abdil Ozdemir²; Jung-Lee Lin³; Chung-Hsuan Chen³; ¹Adapazari, Sakarya; ²Sakarya University, Adapazari, Sakarya; ³Academia Sinica, Taipei, Taiwan
- ThP 612 **Optimization of Proteomic Profiling Approaches for the Cellular Thermal Shift Assay (CETSA) Using Glucosylceramidase-Isofagomine (GBA-IFG) as a Model System**; Clifford Phaneuf¹; PAUL Mason¹; Alexander R. Ivanov²; David Bush³; Alexei Belenky¹; ¹Genzyme, Waltham, ma; ²Northeastern University, Boston, MA; ³Genedata, Lexington, MA
- ThP 613 **Development of Surface Induced Dissociation on a High Mass Range Orbitrap Platform with Applications Toward the Study of Protein Complexes**; Zachary L. VanAernum¹; Joshua D. Gilbert¹; Mikhail E. Belov²; Alexander A. Makarov²; Stevan R. Horning²; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Thermo Fisher Scientific, 28199, Germany
- ThP 614 **A Rapid Mixing Device to Detect Early Intermediates in Hepatitis B Virus Assembly by Charge Detection Mass Spectrometry**; Nicholas Lykтей¹; Corinne Lutowski¹; Zhongchao Zhao¹; Adam Zlotnick¹; Martin Jarrold¹; ¹Indiana University, Bloomington, IN
- ThP 615 **Impact of Charge State on Dissociation of Multimeric Protein Complexes**; Sarah Sipe¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 616 **Enhanced Detection of Non-Covalently Bound Enzyme Complexes Using a Dedicated Large Molecule Autotune on a Q-TOF Mass Spectrometer**; Christian Klein¹; Huiyue Bui¹; Alex Mordehai¹; Caroline S. Chu¹; Gregor Overney¹; William E. Barry¹; ¹Agilent Technologies, Santa Clara, CA
- ThP 617 **Charge State and Stoichiometry Determination for Extremely Congested Mass Spectra of Single- and Mixed-Lipid Membrane Models Using Fourier Analysis**; James S. Prell^{1,2}; Sean P. Cleary¹; ¹Department of Chemistry and Biochemistry, University of Oregon, Eugene, OR; ²Materials Science Institute, University of Oregon, Eugene, OR
- ThP 618 **Untargeted Characterization of Protein Complex Stoichiometry and Cofactor Binding with Native Proteomics**; Owen Skinner¹; Nicole A Haverland¹; Luca Fornelli¹; Rafael D Melani¹; Luis H. F. Do Vale^{1,2}; Henrique S Seckler¹; Peter F Doubleday¹; Luis F Schachner¹; Kristina Srzentic¹; Neil L Kelleher¹; Philip D Compton¹; ¹Northwestern University, Evanston, IL; ²University of Brasilia, Brasilia, Brazil
- ThP 619 **Functional Analysis of Soluble and Membrane-Associated Protein Complexes by Multi-Dimensional Protein Correlation Profiling**; Zach McBride¹; Donglai Chen²; Jun Xie²; Daniel Szymanski²; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, Indiana
- ThP 620 **LC-MS Compatible Sample Preparation Using On-bead Digestion to Characterize Protein-Protein Interactions in Early Mouse Embryonic Cortical Development**; Philip Loziuk¹; Caroline Johnson²; Troy Ghashghaei²; ¹North Carolina State University, Raleigh, NC; ²North Carolina State University, Raleigh, NC
- ThP 621 **A Modified flow-FPOP Platform for Oxidative Footprinting of Size-Fractionated Complexes**; Manolo D. Plasencia¹; Don L. Rempel²; Michael L. Gross²; ¹University of Michigan, Ann Arbor, MI; ²Washington University, St. Louis, MO
- ThP 622 **Native LESA Mass Spectrometry: Direct Analysis of Proteins and their Complexes**; Rian L. Griffiths¹; Victor A. Mikhailov²; Emma K. Sisley¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, UK; ²University of Oxford, Oxford, UK
- ThP 623 **Native Mass Spectrometry Measurements Directly from Crude Cell Lysates**; Jinrui Gan¹; Gili Ben-Nissan¹; Galina Arkind¹; Mark Tarnavsky¹; Devin Trudeau¹; Lianet Noda Garcia¹; Dan S. Tawfik¹; Michal Sharon¹; ¹Weizmann Institute of Science, Rehovot, Rehovot
- ThP 624 **Deconvolving Extremely Congested Mass Spectra of Nanodisc Membrane Models and Polymers Using Overtone Data from Fourier Transformed Spectra**; Sean P. Cleary¹; James S. Prell^{1,2}; ¹Department of Chemistry and Biochemistry, University of Oregon, Eugene, OR; ²Materials Science Institute, University of Oregon, Eugene, OR
- ThP 625 **Cryogenic Ion Mobility-Mass Spectrometry Directly Observes Dimer Dehydration of Insulin**; Michael J. Hebert¹; David H Russell¹; ¹Texas A&M University, College Station, TX
- ThP 626 **Evaluation for the Need of Adequate Sample Size for Affinity Purification-Mass Spectrometry**; Pamela S. Cantrell¹; Mai Sun¹; Nathan A. Yates^{1,2}; Xuemei Zeng¹; ¹Biomedical Mass Spectrometry Center, University of Pittsburgh Health Sciences Core Research Facilities, Pittsburgh, PA; ²University of Pittsburgh School of Medicine, Pittsburgh, PA
- ThP 627 **Combining Native Mass Spectrometry with Mechanistic Binding Models to Define Microscopic Thermodynamics of Homotropic Allostery in Oligomeric Proteins**; Melody Holmquist¹; Bryant Jacob¹; Eilhu C. Ihms¹; Paul Gollnick²; Vicki H. Wysocki¹; Mark P. Foster¹; ¹The Ohio State University, Columbus, OH; ²University at Buffalo, Buffalo, NY
- ThP 628 **Developing LC-MS Methods to Characterize the Interaction of Therapeutic Proteins with Heparin Oligosaccharides**; Cedric E. Bobst¹; Igor A. Kaltashov²; ¹University of Massachusetts, Amherst, MA; ²University of Massachusetts Amherst, Amherst, MA

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- ThP 629 **Cytochrome c as a Peroxidase: Covalent Labeling and Oxidation Site Mapping Uncovers the Mechanism of Catalytic Activation by H₂O₂**; Victor Yin¹; Gary S Shaw¹; Lars Konermann¹; ¹University of Western Ontario, London, ON, Canada
- ThP 630 **Quantitative Crosslinking and Quantitative Surface Modification for the Structural Characterization of Disorder-To-Order Transitions**; Karl A.T. Makepeace¹; Evgeniy V. Petrotchenko²; Christoph H. Borchers^{1,2}; ¹Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ²University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada
- ThP 631 **Structural Mapping of Atypical Chemokine Receptor 3 by Mass Spectrometry**; Liwen Wang¹; Martin Gustavsson²; Tracy Handel²; Irina Kufareva²; Mark R. Chance¹; ¹Case Western Reserve Univ, Cleveland, OH; ²University of California San Diego, San Diego, CA
- ThP 632 **The Aggregation Mechanism of a Naturally Occurring Highly Amyloidogenic β 2-Microglobulin Variant Probed Using Structural Mass Spectrometry**; Owen Cornwell¹; Sheena E Radford¹; Alison E Ashcroft¹; ¹University of Leeds, Leeds, Yorkshire
- ThP 633 **Proteolytic MALDI Compatible Chips for Limited Proteolysis and H/D Exchange Analysis**; Michal Rosulek^{1,2}; Petra Darebna^{1,2}; Lukas Slavata^{1,2}; Michael Volny³; Petr Man^{1,2}; Petr Pompach^{1,3}; Petr Novak^{1,2}; ¹BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; ²Faculty of Science, Charles University, Prague, Czech Republic; ³Affipro s.r.o., Mratin, Czech Republic



- ThP 634 **The C-type Lectin-Like Receptor Nkrp1b: Important Structural Features in the Context of Protein Conformation and Interactions;** Lucie Hernychova^{1,2}; Michal Rosulek^{2,3}; Ljubina Ivanova²; Valeria Grobarova¹; Ondrej Sebesta¹; Alan Kadek^{2,3}; Josef Chmelik⁴; Kristian Skala²; Zdenek Kukacka^{2,3}; Jan Cerny¹; Petr Novak^{2,3}; ¹Department of Cell Biology, Faculty of Science, Charles University, Prague, Czech Republic; ²BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; ³Department of Biochemistry, Faculty of Science, Charles University, Prague, Czech Republic; ⁴Institute of Microbiology of the CAS, v.v.i., Prague, Czech Republic
- ThP 635 **Utilizing 193 nm UVPD for Identification of Peptide Crosslinks to Characterize Protein Interactions;** Michael Cammarata¹; Sarah Sipe¹; Jake Rosenberg¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 636 **Structural Characterization of Protein by Using Enzymatic Reactor;** Griffee Elodie¹; Hanozin Emeline¹; Smargiasso Nicolas¹; Quinton Loïc¹; Mazzucchelli Gabriel¹; De Pauw Edwin¹; ¹Mass Spectrometry Laboratory, Liège, Belgium
- ThP 637 **Complex Conformations: Ion Mobility Mass Spectrometry Provides Insight into a Conformationally Dynamic Protein Complex;** Sophie R Harvey¹; Varun V Gadkari¹; Zucal Suo¹; Vicki H Wysocki¹; ¹The Ohio State University, Columbus, OH
- ThP 638 **Exploring Two-State Cooperative Protein Folding Using Ion Mobility Spectrometry-Mass Spectrometry;** Shannon A Raab¹; Tarick J El-Baba¹; Daniel W Woodall¹; Wen Liu²; Yang Liu²; Arthur Laganowsky²; David H Russell²; David E Clemmer¹; ¹Indiana University, Bloomington, IN; ²Texas A&M University, College Station, Texas
- ThP 639 **Probing Ligand-Induced GPCR Conformational Changes by In-Cell Crosslinking and Mass Spectrometry** ; Bill Huang¹; Ji-Won Lee¹; Hee-Yong Kim¹; ¹NIAAA/NIH, Rockville, MD
- ThP 640 **Structural Comparisons of Trimeric Phospholipase A2 from Australian Snake Venoms;** Julian A. Harrison^{1,2}; Celine Kelson^{1,2}; Jenny L. Beck^{1,2}; ¹School of Chemistry, University of Wollongong, Wollongong, Australia; ²Illawarra Health and Medical Research Institute, University of Wollongong, Wollongong, Australia
- ThP 641 **Investigating the Dynamics and Assembly of alpha-Synuclein Amyloid Oligomers by ESI-IMS-MS;** Rebecca Mason¹; Caroline Dalton¹; David Smith¹; ¹Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, UK
- ThP 642 **Quantitative Protein Topography Measurements by High Resolution Hydroxyl Radical Protein Footprinting for Molecular Modeling;** Boer Xie¹; Amika Sood¹; Robert J. Woods¹; Joshua S. Sharp²; ¹Complex Carbohydrate Research Center, University of Georgia, Athens, GA; ²University of Mississippi, University, MS
- ThP 643 **Integrative MS-based Biophysical Methods Show the Bridging Two Domains is a Mechanism for catalysis of OCP by FRP;** Yue Lu; Washington University, St. Louis, St Louis
- ThP 644 **Delivering Transmembrane Peptide Complexes to the Gas Phase Using ESI and Nanodiscs;** Jun Li¹; Michele R. Richards¹; Elena Kitova¹; John Klassen¹; ¹University of Alberta, Edmonton, AB, Canada
- ThP 645 **Advancing Synchrotron X-Ray Protein Footprinting through Radiolysis Chemistry and Post-Exposure Treatments;** Simin D. Maleknia¹; Sayan Gupta²; Corie Ralston²; ¹University of New South Wales, Sydney , NSW; ²Lawrence Berkeley National Laboratory, Berkeley, CA
- ThP 646 **Proteome Thermostability in the Bacillaceae Family;** Jeremy Volkening¹; Pei Liu¹; Greg Sabat¹; Michael R. Sussman¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 647 **Epitope and Paratope Mapping of Virus-Antibody Complexes;** Ganesh S. Anand¹; Xin Xiang Lim²; Arun

Chandramohan²; ¹NUS Singapore, Singapore; ²National University of Singapore, Singapore, Singapore

- ThP 648 **A Traveling Wave Ion Mobility Spectrometry and Molecular Modeling Study of Heparin/HS-Protein Interactions for Robo1;** Yuejie Zhao¹; Jeong Yeh Yang²; Yongmei Xu³; David Thieker²; Chengli Zong²; Kelley Moremen²; Jian Liu³; Geert-Jan Boons²; Robert Woods²; I. Jonathan Amster¹; ¹University of Georgia, Chemistry Department, Athens, GA; ²Complex Carbohydrate Research Center, University of Georgia, Athens, GA; ³University of North Carolina, Chapel Hill, NC

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- ThP 649 **High Resolution Protein Profiling of Aortic Valves with and without Left-Ventricular Assist Device (LVAD) Implantation;** Hemanth Akkiraju¹; Lewis M. Brown¹; Elizabeth H. Stephens¹; Jiho Han¹; Emma Trawick¹; Gordana Vunjak-Novakovic¹; Hiroo Takayama¹; ¹Columbia University, New York , NY
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- ThP 651 **Phospho-Barcodes of Renal Cell Carcinoma Cell Lines Reveals Differential Mechanisms in Sunitinib Resistance;** Shao-Kuan Chen^{1,2}; Chi-Jung Huang^{2,3}; Yen-Chieh Wang^{1,2}; Tai-Yuan Lin¹; Wei-Chi Ku¹; ¹fu Jen Catholic University, New Taipei City, Taiwan; ²Cathay General Hospital, Taipei, Taiwan; ³National Defense Medical Center, Taipei, Taiwan
- ThP 652 **Forensic Proteomics – Identification of an Unknown Snake Venom in a Post-Mortem Blood Sample;** Kyung-Mee Moon¹; Jason Rogalski¹; Leonard Foster¹; ¹University of British Columbia, Vancouver, BC, Canada
- ThP 653 **Proteomes of Paired Human Plasma and Cerebrospinal Fluid and their Association with Protein Biomarkers of Alzheimer's Disease;** Loïc Dayon¹; Jérôme Wojcik²; Antonio Núñez Galindo¹; John Cortésy¹; Ornella Cominetti¹; Domilė Tautvydaitė³; Aikaterini Oikonomidi³; Hugues Henry⁴; Martin Kussmann¹; India Severin¹; Eugenia Migliavacca¹; Gene L. Bowman¹; Julius Popp^{3,5}; ¹Nestlé Institute of Health Sciences, Lausanne, Switzerland; ²Quartz Bio, Geneva, Switzerland; ³CHUV, Old Age Psychiatry, Department of Psychiatry, Lausanne, Switzerland; ⁴CHUV, Department of Laboratories, Lausanne, Switzerland; ⁵CHUV, Leenaards Memory Center, Department of Clinical Neurosciences, Lausanne, Switzerland
- ThP 654 **Immuno-MALDI for Quantifying Signaling Pathway Activity;** Robert Popp¹; Huiyan Li¹; Andrew G. Chambers¹; Adriana Aguilar-Mahecha²; Oliver Pötz³; Mark Basik⁴; Christoph H. Borchers^{1,4,5}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Segal Cancer Center, McGill University, Montreal, QC, Canada; ³Natural and Medical Sciences Institute (NMI), University of Tübingen, Reutlingen, Germany; ⁴Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada; ⁵Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
- ThP 655 **De Novo Sequencing Of Multiple Myeloma Immunoglobulin Heavy Chain CDR3 Clone From A Polyclonal Background;** David H. Tse^{1,2}; Benson M. Linda^{1,3}; Benjamin J. Madden^{1,3}; Renee C. Tschumper^{1,4}; Diane F. Jelinek^{1,4}; Angela Dispenzieri^{1,5}; K. Ilker Sen⁶; Baozhen Shan⁷; H. Robert Bergen, III^{1,2,3}; ¹Mayo Clinic, Rochester, MN; ²Dept. of Biochemistry and Molecular Biology, Rochester, MN; ³Mayo Proteomics Research Core, Rochester, MN; ⁴Dept. of Immunology, Rochester, MN; ⁵Dept. of Hematology, Rochester, MN; ⁶Protein Metrics Inc., San Carlos, CA; ⁷Bioinformatics Solutions Inc, Waterloo, ON, Canada



- ThP 656 **A Novel Data Independent Acquisition Method for Hemoglobin Variant Identification in Clinical Research;** Jonathan P. Williams¹; Christopher J. Hughes¹; Heather A. Brown¹; Keith Richardson¹; Johannes P.C. Vissers¹; ¹Waters Wilmslow UK, Wilmslow, Cheshire
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- ThP 659 **PeptideMapper: an Integrated Resource for Targeted Proteomics;** Pallab Bhowmick¹; Yassene Mohammed^{1,2}; Christoph H. Borchers^{1,3,4}; ¹University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; ²Center for Proteomics and Metabolomics, Leiden University, Netherlands; ³Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; ⁴Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada
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- ThP 677 **Mass Spectrometry of DNA-Protein Cross-Links Following Ischemia-Reperfusion Injury;** Natalia Tretyakova¹; Arnold Groehler IV¹; Qinglu Li¹; Mary G. Garry¹; ¹University of Minnesota, Minneapolis, MN



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- ThP 697 **Proteomic Analysis Reveals Role of the Phosphohistidine Phosphatase PHPT1 in Ethanol-Induced Hepatic Steatosis**; Daniel Martin¹; Crystina Kriss¹; Catherine MarElia¹; Brant Burkhardt¹; Stanley M. Stevens¹; ¹University of South Florida, Tampa, FL
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