

71ST CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS

June 4 - 8, 2023 | Houston, Texas



SHORT COURSES June 3 & 4

George R. Brown Convention Center

#ASMS2023



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Welcome to the 71st ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the George R. Brown Convention Center. Corporate Hospitality Suites are at the Hilton Americas.



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PROGRAM HIGHLIGHTS

BADGE PRINTING 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, Hall B3 Plan Your Strategy: What to See and Do at ASMS

SUNDAY TUTORIAL SESSION I,

Hall B3 5:00 – 5:45 pm Mass Spectrometry and Medicine

Livia Eberlin

Medicine

Baylor College of

SUNDAY TUTORIAL SESSION II, Ballroom A 5:00 – 5:45 pm Mass Spectrometry and

Anti-Doping Research Mario Thevis



Center for Preventive Doping Research, German Sport University Cologne

SUNDAY SPECIAL KEYNOTE SESSION 5:45 - 6:30 PM, Hall B3



Jeremy Edwards Chair, Houston LGBTQ Advisory Committee

Activism in Houston - Boots on the Ground: Progress & Challenges

SUNDAY CONFERENCE OPENING 6:45 - 7:45 PM, Hall B3



Welcome

Joseph A. Loo *University of California, Los Angeles* ASMS Vice President for Programs



From Human Genome Project to Precision Medicine - A Journey in Chemistry and Technology

Richard A. Gibbs Baylor College of Medicine

SUNDAY WELCOME RECEPTION 7:45 - 9:00 PM

Posters-Exhibits Hall (Level One). Conference name badge is required.

Consult online planner or mobile app for detailed program.

MONDAY AWARD LECTURE 4:45 - 5:30 PM, Hall B3



John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

Carol V. Robinson University of Oxford

TUESDAY AWARD LECTURE 4:45 - 5:30 PM, Hall B3



Biemann Medal

Brandon Ruotolo University of Michigan

Wednesday ASMS Meeting 4:45 - 5:30 PM, Hall B3

Enjoy a beverage, hear ASMS Board reports and applaud award recipients.

THURSDAY PLENARY SESSION 4:45 - 5:30 PM, Hall B3



The Rise and Reign of the Mammals: A New History, from the Shadow of the Dinosaurs to Us

Stephen Brusatte University of Edinburgh

THURSDAY CLOSING EVENT Advance Purchase Ticket Required Ticket Sales Close at 12pm (noon), Monday, June 5

Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.



The event is at the Houston Museum of Natural Science on Thursday, June 8, 7:00 - 10:00 pm. Buffet dinner is included. Cash

bars available. Enjoy the INCREDIBLE paleontology and gem exhibitions at the museum. Closing plenary speaker, Steve Brusatte, will attend the event and provide additional Q&A in the Morian Hall of Paleontology.

There is no organized transportation to/from the event. Attendees with the closing event icon on their badge have round-trip light rail included. Please wear your badge in case there is ticket control. Engineers will identify your closing event icon as your paid ride. Light rail instructions are included in the app and will be emailed to all who have purchased the closing event.

The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030.

If you do not wish to take the light rail, Uber/Lyft or taxis are available at standard rates.



ORAL SESSIONS are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday. All session rooms are on Level Three.

ORAL PRESENTATIONS. Speakers are required to use the ASMS computers for their presentations. ASMS will have a PC and MAC available in each session room for presentations.

SPEAKERS must load presentations at least one day prior to their talks. The speaker ready room is Room 330 AB. The room is open with a technician according to this schedule:

Sunday 10:00 am - 8:00 pm Monday through Wednesday 7:30 am - 6:00 pm Thursday 7:30 am - 2:30 pm

POSTERS AND EXHIBIT BOOTHS, Halls BC (Level One). The Hall is open:

find exhibit booths staffed 9am-2pm

POSTER SET-UP is by 8:30 am on the day scheduled. A counter for poster supplies is inside the main entrance to the Hall (Level One).

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. This schedule allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors are welcome to attend the full four hours).

Odd-number posters present:

10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:

10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm.

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 be removed between 7:00-8:00 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.

WORKSHOPS are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided.

FREE WIFI Access is available throughout the convention center, look for the ASMS network on your device and use password *asms2023*.

CAREER CENTER is located in Room 352DEF (Level Three). 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 are available nearby and should be reserved one-day in advance.

Sunday	7:45 -	9:00 pm
Monday - Wednesday7	:30 am -	5:00 pm
Thursday7	:30 am -	2:30 pm

GENDER NEUTRAL RESTROOMS locations throughout the convention center. Please ask at the Information counter near badge printing on Level One if you need assistance finding these locations.

MOTHER'S LOUNGE is available for use by nursing mothers. For location, please consult General Information in mobile app or ask at the Information counter near badge printing on Level One.

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CODE OF CONDUCT

The ASMS Code of Conduct guides the expected, professional behavior of all participants at conferences, short courses, and conference-related activities and events.

ACCEPTABLE BEHAVIOR INCLUDES:

- Treating everyone with respect and consideration;
- Communicating openly and thoughtfully with others and being considerate of the multitude of views and opinions that may be different from your own;
- · Being respectful and mindful in your critique of ideas;
- Being mindful of your surroundings and of your fellow participants.

UNACCEPTABLE BEHAVIOR INCLUDES:

- Harassment and intimidation, including any verbal, written, or physical conduct designed to threaten, intimidate, or coerce any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Discrimination based on gender or gender identity, sexual orientation, age, disability, physical appearance, body size, race, religion, national origin, culture, or any other characteristic provided by law;
- Physical or verbal abuse of any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Threats of physical violence against any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest; and
- · Disrespectful disruption of presentations.

CONSEQUENCES OF UNACCEPTABLE BEHAVIOR:

Anyone who violates this Code may be subject to the consequences. ASMS reserves the right to take action beyond these consequences as necessary based on a participant's behavior in violation of the Code.

- Anyone requested to stop unacceptable behavior is expected to comply immediately;
- Immediate removal from the meeting or event without warning and potentially without refund; and/or
- Prohibition from attending future meetings or events in the sole determination of ASMS.

Who to contact:

ASMS Executive Director, Jennifer Watson, jennifer@asms.org

ASMS is proud of our annual conferences, short courses, and conference-related events and wants everyone to have a positive learning and networking experience. Embracing the above professional behavior will help ensure a great experience for all involved.

Text adapted from https://www.frontiersin.org/articles/10.3389/ fmars.2016.00103/full

Favaro Brett, Oester Samantha, Cigliano John A., Cornick Leslie A., Hind Edward J., Parsons E. C. M., Woodbury Tracey J., "Your Science Conference Should Have a Code of Conduct", Frontiers in Marine Science, 2016, 3, 103

CONFERENCE REGULATIONS

Name badge is required for all conference sessions, short courses, and conference-related events (hospitality suites, closing event.)

All devices must be silenced and screens darkened in oral sessions.

No photography or recording is allowed in oral sessions or in the poster hall.

Publicity Release. By attending or participating in an ASMS event, attendees agree to allow their names, likenesses, and images, in audio, photographic or video format recorded for the event and onsite, to be used by ASMS for educational, promotional, or marketing of ASMS events or activities.

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. If you wish to cite an abstract presented at the annual conference, please use the citation guidelines for conference proceedings found at asms.org.

The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. Ask at Registration desk to have your announcement approved.

Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.

No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).

Corporate 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 are permitted.

In general, ASMS provides the following advice for parents considering bringing child(ren) or infant(s): Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices are permitted in the poster hall, and with careful supervision by parents. Strollers are prohibited in the hospitality suites.

Consult online planner or mobile app for detailed program.



INFORMATICS HUB

Inside the Poster/Exhibit Hall daily during poster sessions.

The Informatics Hub is a place where informaticians gather with three aims:

- 1. to provide their advice, knowledge, and support to ANYONE with a relevant question;
- to discuss current issues and challenges in mass spectrometry informatics with the entire community;
- 3. to work on interesting, synergistic projects and to freely exchange tools, algorithms, and knowhow with each other, across all labs, seniorities and levels of experience.

SPECIAL 3D PRINT DISPLAY Inside the Poster/Exhibit Hall

Get inspired for your own design and access useful design files from your colleagues. 3D prints on display represent:

- MS Parts
- LC and other Labware
- Educational items



NETWORKING OPPORTUNITIES

Special Gap Hour Receptions

Monday, Tuesday & Wednesday 7:00-8:00 PM

Monday, 7pm / Ballroom B Sponsored by Agilent

Reception immediately following workshop 06 Networking for Scientists: Celebrating Women Mass Spectrometrists. All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.

Tuesday, 7pm / Ballroom B Sponsored by SCIEX

Reception immediately following workshop 06 Recognizing the "A" in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists. All are welcome to join for networking focused on accessibility, diversity, and inclusion.

Wednesday, 7pm | Ballroom B Sponsored by SEER

Reception immediately following workshop 06 MS Career Options: How to Kick Start Your Career. All are welcome to join for networking focused on career development.

LOOK

Main foyer near entrance to Posters/Exhibit Hall.



Funding Agency Office Hours

Inside Posters/Exhibit Hall Monday-

Thursday 10:30 am - 2:30 pm. Meet with representatives from various funding agencies. Appointment sign-up sheets will be posted on 'office' entry sign (along main entry inside posters-exhibits area).

Attendees are encouraged to take advantage of this valuable resource while at the conference.

ASMS BOARD OF DIRECTORS





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Member-at-Large for Publications Stephen Valentine West Virginia University Morgantown, PA

CONGRATULATIONS

to these members who are elected to serve on the ASMS Board. Their terms begin July 1, 2023

Vice President for Arrangements



Patrick Batoon Agilent Technologies Santa Clara, CA

Secretary



Stephanie M. Cologna University of Illinois Chicago Chicago, IL

Member-at-Large for Publicatins



Kelly M. Hines University of Georgia Athens, GA



INTEREST GRO	UP COORDINATORS	Polymeric Materi	als Thierry Fouquet
Ambient Sampling and Ionization	Anyin Li Chris Gill	Regulated Bioanaly	Anthony Gies sis Wenkui Liu
Analytical Laboratory Managers	Brett Phinney Uri Keshet	Top-Down Proteom	Jian Wang ics Yuri E.M. van der Burgt
Bioinformatics for MS	Katarzyna Kulej Claire O'Donovan	Undergradua	Mowei Zhou ate Brandie Ehrmann
Biotherapeutics	Andrew Mahan Da Ren	Research in N Young Ma	//S Mac Gilliland Iss Ryan Bain
Career Development	Elizabeth Pierson Troy D. Wood	Spectrometri	sts Christopher Pulliam
Clinical Chemistry	Brian Rappold	Asilomor	Committees
Data Independent Acquisition	Lindsay Pino Lukas Reiter	Conference (ACMS)	Jason Hogan Laura Sanchez
Developing World Research & Educ.	Giles Edwards Kym Faull	Audit	Susan Richardson (ASMS Board Rep.) Ying Ge, Chair
Drug Metabolism & Pharmacokinetics	Lina Luo Hlaing (Holly) Maw		Kevin Bateman Ljiliana Pasa-Tolic Sharan Bittari (ASMS Tragguran)
Energy, Petroleum & Biofuels	Yuri Corilo Leonard Nyadong	Corporate	Michael Easterling (ASMS Board Rep)
Environmental Applications	Ahmed Hamid Kevin Tucker	Liaison	Angie Jinks, Thermo Fisher Scientific Melanie Juba, SCIEX
Exposomics	Benedikt Warth Ruth Marfil-Vega		Lance Nicolaysen, Waters Corporation Bruce Peat, Peak Scientific
Flavor, Fragrance and Foodstuff	Joe Binkley Liz Humston-Fulmer	Digital	St John Skilton, Protein Metrics Birgit Schilling, Chair
Forensics & Homeland Security	J. Tyler Davidson Ruth Smith Waddell	Communications	Chris Chouinard Lauren Stopfer Thomas Wales
FTMS	David Butcher Yuri Corilo	Membershin Diversity	Susan Richardson (ASMS Board Rep)
Fundamentals	Alexander Makarov Yury Tsybin	and Inclusion	Saiful Chowdhury Dominic Gostick
Imaging MS	Ingela Lanekoff Boone Prentice		Hee-Yong Kim Baljit Ubhi
Ion Mobility MS	James Prell Xueyun Zheng	Education	Livia Eberlin, Chair Joseph Eschweiler Lisa O'Callaghan
Ion Trap MS	Dalton Snyder Lucas Szalwinski		Stacy Malaker lan Webb
LC/MS Related Topics	James Dodds Jack Ryan	History	P. Jane Gale, Chair Catherine Fenselau
Lipids & Lipodomics	Michael Holčapek Harold Köfeler		David Herold Asher Newsome
Mass Spectral Libraries	Emma Rennie Xiaoyu (Sara) Yang	Nominating	Michael Grayson, <i>ex-officio</i>
Metabolomics	Maryam Goudarzi Thomas Horvath Tytus Mak	Nominaung	Peggi Angel Tarun Anumol Abraham Badu-Tawiah
Native MS	Justin Benesch Arthur Laganowsky Kristine Parson	Publications	Touradji Solouki Stephen Valentine, Chair
Oligonucleotides & Nucleic Acids	Varun Gadkari Jennifer Lippens Robert Ross		Joe Cannon Vanessa Phelan Stefanie Thomas Mowei Zhou Vicki Wysocki. <i>ex officio</i>
	Kiran iyer Jeremy Manheim	Sanibel	Richard Rogers, Chair
Photoionization MS	Luke Hanley Christopher Rueger	Conterence	Sarah Rogstad Sharon Pitteri (ASMS Board Rep.)

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71ST ASMS CONFERENCE ON MASS SPECTROMETRY



JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY 2023 Recipient: Carol V. Robinson Award Lecture: 4:45 PM, Monday, Hall B3



The ASMS Award for Distinguished Contribution in Mass Spectrometry honors the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray ionization. The award is conferred at the ASMS Annual Conference with the presentation of a \$10,000 cash award, a recognition plaque, and the award lecture.

Carol V. Robinson is the recipient of the 2023 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry for the development of mass spectrometry methods for the analysis and characterization of membrane proteins. Dr. Robinson's pioneering contributions have improved our fundamental understanding of membrane protein complex structure and the role of lipid binding in membrane protein function. Her work has

enabled new knowledge into disease mechanisms and has had tremendous impact in drug discovery. Specific accomplishments include: (1) pioneering development of methods to enable gas phase analysis of membrane protein complexes; (2) the application of ion mobility MS and collision-induced unfolding methods to investigate lipid-membrane protein binding; (3) the application of high-resolution MS to resolve the complexity of lipid-protein binding events; and (4) the innovative development of methods for native analysis of membrane protein complexes and lipid binding.

Her collective achievements have been amplified by her dedication to the dissemination of detailed protocols and troubleshooting advice to the research community – ensuring that others had the necessary information to implement the methods. This outreach has resulted in an active cohort of MS researchers across the globe working on the mass spectrometry of membrane protein complexes.

In 2013 Carol was elevated to the title of "Dame Commander of the Order of the British Empire (DBE)" for services to science and Industry. Professor Dame Carol Robinson is University Chair and Professor of Chemistry, University of Oxford.



BIEMANN MEDAL 2023 Recipient: Brandon Ruotolo Award Lecture: 4:45 PM, Tuesday, Hall B3



The Biemann Medal is awarded to recognize significant achievement in basic or applied mass spectrometry in the early stages of an academic career. The Medal is conferred at the ASMS Annual Conference with the presentation of a \$5,000 cash award and the award lecture.

Brandon Ruotolo is the recipient of the 2023 ASMS Biemann Medal for his significant contributions in the development and application of novel high performance mass spectrometry technologies for protein and protein complex structure elucidation. Examples of his innovative scientific contributions include: (1) leadership in the development of ion mobility MS (IM-MS) for structural characterization of biopolymers; (2) refinement of collision induced unfolding (CIU) methods that enable determination of the number of autonomously folded domains

within proteins and characterization of stability reflective of changes in both local and global protein structure; (3) the use of CIU to probe the relative stability of protein-ligand interactions; (4) the development of chemical cross-linkers to stabilize protein structure in the absence of bulk solvent; (5) integration of IM-MS and other structural MS methods as a high-throughput approach for structural proteomics; and (6) application of IM-MS as a screening tool for therapeutic drug discovery. Dr. Ruotolo has built an impressive research program that is addressing application of high impact to the biology and medical communities.

Dr. Ruotolo is Professor of Chemistry, University of Michigan.



AL YERGY MS SCIENTIST AWARDS 2023 Recipients Award Presentations: 4:45 PM, Monday, Hall B3

The AI Yergey MS Scientist Awards are sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes." The awards are named in memory of AI Yergey a well-respected scientist who was known as a dedicated mentor. Each award is conferred at the ASMS Annual Conference with \$1,000 cash award and a recognition memento.



Eduard Denisov (Thermo Fisher Scientific) is one of key people whose hard and creative work over the last two decades was crucial for making Orbitrap mass spectrometry the leading technique in high resolution mass spectrometry. He took a leading part in experimental development of all major elements of the Orbitrap technology. Over all these years he remained a reliable, modest and at the same time a very passionate enthusiast of Orbitrap technology, who really cares that every user of this technology is getting the best results.



Jodie Johnson (University of Florida) is so extremely valuable to MSREC, the University of Florida, and the larger MS community. No matter where you are in your MS career, from novice to 20 years of experience, one can learn invaluable knowledge from Dr. Johnson. He is a dedicated mentor and his knowledge is expansive in areas of chromatography and mass spectrometry. He loves to share his knowledge and loves to engage in research discussions.



Amina Woods (NIDA IRP, NIH) has made significant contributions to MS-based science and her dedication to the field of mass spectrometry is amply featured by her record of research, service and teaching. Amina has willingly offered her knowledge through many venues. Biological mass spectrometry became an integral component of her research activities in the early 1990s when she became affiliated with the late Bob Cotter using plasma desorption MS to characterize biological molecules. From then on, mass spectrometry has been at the heart of much of her research portfolio and her community participation in many mass spectrometry organizations including ASMS.

RON HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS Award Presentation: ASMS Meeting, 4:45 PM, Wednesday, Hall B3

The Ron Hites Award recognizes an outstanding publication of original research published in JASMS. 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 plaque for principal author and certificates for co-authors.



Joshua Sharp (University of Mississippi) is recipient of the 2023 Hites Award along with co-authors Emily E. Chea, Sandeep K. Misra, Ron Orlando, Marla Popov, Robert W. Egan, David Holman, and Scot R. Weinberger for their paper "Flash Oxidation (FOX) System: A Novel Laser-Free Fast Photochemical Oxidation Protein Footprinting Platform", 2021, **32**, 1601-1609.



2023 RESEARCH AWARDS Award Presentations: 4:45 PM, Tuesday, Hall B3

Research Awards promote the research of academic scientists within the first four years of joining the tenure track or research faculty of a North American University at the time the award is conferred. The awards, in the amount of \$35,000 for the recipient's proposed research are fully funded by Bruker, Thermo Fisher Scientific, and Waters Corporation and are made to the institution of each recipient.



Funded by

Kelly Marie Hines University of Georgia





Jesse Meyer Cedars-Sinai Medical Center



Funded by Waters

Stacy Malaker Yale University

Research At Primarily Undergraduate Institution (PUI) Award Award Presentation: 4:45 PM, Tuesday, Hall B3





This award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The Award of \$20,000 for the recipient's proposed research is fully funded by Agilent and is made to recipient's institution.

Erica Jacobs St. Johns University



2023 POSTDOCTORAL CAREER DEVELOPMENT AWARDS Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Hall B3

Postdoctoral Career Development Awards in the amount of \$5,000 promote professional career development of postdoctoral fellows in the field of mass spectrometry.



Emma Guiberson Stanford University



Haiyan Lu University of Wisconsin-Madison



Melanie Odenkirk Colorado State University



Suttipong Suttapitugsakul Beth Israel Deaconess Medical Center



Yixuan Xie Washington University School of Medicine

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2023 GRADUATE STUDENT TRAVEL AWARDS Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Hall B3

Elizabeth Bayne University of Wisconsin-Madison

Danielle Caefer University of Connecticut

Hsin-Hsiang Chung National Taiwan University Steven DeFiglia

University of Michigan

Sarah Dowling Indiana University-Purdue University Indianapolis

Kimberly Fabijanczuk *Purdue University*

Ashley Frankenfield George Washington University Viraj Gandhi Indiana University-Purdue University Indianapolis

Yanting Guo University of Oklahoma

Amanda Khoo University of Toronto David Koomen

Vanderbilt University Nicolas Morato

Dinuri Fernando

Purdue University Leena Pade

University of Maryland-College Park Austin Salome University of Wisconsin-Madison Madison Turner University of Guelph Benqian Wei

University of California, Los Angeles

David Williamson University of Utah

Tingyuan Yang Texas A&M University Kejun Yin

Georgia Institute of Technology

2023 UNDERGRADUATE STUDENT TRAVEL AWARDS Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Hall B3

Megan Bindra Saint Mary's College of California Emily Boyette South Florida State College Olivia Dioli North Carolina State University Celine Ertekin University of California, Santa Cruz

University of North Carolina, Chapel Hill Yu Tin Lin Univeristy of Florida Lawren Paris University of Oregon Aliyah Remoroza University of Maryland Baltimore County Philenroza Thavrin Oregon State University Oliver Wu University of Oklahoma





LEVEL THREE



LEVEL TWO





- X-



POSTER-EXHIBIT HALL



GEORGE R. BROWN CONVENTION CENTER

*





DOWNTOWN HOTELS

- Aloft Houston Downtown
 0.5 miles 15 min. walk
- Cambria
 0.6 miles 15 min. walk
- Courtyard by Marriott
 0.5 miles 15 min. walk
- 4. Embassy Suites Hotel 0.3 miles — 10 min. walk
- 5. Four Seasons 0.5 miles — 15 min. walk

- Hampton Inn
 0.3 miles 10 min. walk
- 7. Hilton Americas Houston Connected to GRB via Skybridge
- Homewood Suites
 0.3 miles 10 min. walk
- 9. Le Meridien 0.5 miles — 15 min. walk

- 10. Marriott Marquis Connected to GRB via Skybridge
- 11. Residence Inn Houston 0.6 miles — 15 min. walk
- 12. Springhill Suites 0.6 miles — 15 min. walk
- 13. The Laura 0.5 miles — 15 min. walk



X

Escalator Elevator



MEDIA EVENTS (PRESS CONFERENCES) AT HILTON AMERICAS

All members of the press are invited to attend these events at the Hilton Americas.

MONDAY, JUNE 5			
Time	Company	Hilton Americas	
8:00 – 9:00 am	Shimadzu	Grand Ballroom GHI	
9:30 - 10:30 am	Bruker Daltonics	Americas Ballroom AB	
11:00 am - 12:00 pm	SCIEX	Grand Ballroom JKL	
1:30 - 2:30 pm	Agilent	Americas Ballroom EF	
3:00 – 4:00 pm	Thermo Fisher Scientific	Grand Ballroom ABC	
4:30 - 5:30 pm	Waters	Grand Ballroom DEF	

BREAKFAST SEMINARS AT CONVENTION CENTER & HILTON AMERICAS

Breakfast Seminars are hosted by Corporate Members at the George R. Brown Convention Center and the Hilton Americas. Pre-registration (RSVP) is recommended. Please look for Breakfast Seminars page on www.asms.org and in the online planner / mobile app to find online registration links for these events.

MONDAY, JUNE 5 / All breakfasts begin at 7:00 AM					
George R. Brown	Convei	ntion Center		Hilton	Americas
908 Devices	Room	342 AB		Agilent	Americas Ballroom EF
ACD/Labs	Room	371 CF		MOBILion Systems	Room 335 A
Agilent	Room	320 A		SCIEX	Grand Ballroom JKI
Biognosve	Room	361 ABDE		Shimadzu	Grand Ballroom GHI
Diognosys	-			Thermo Fisher Scientific	Grand Ballroom ABC
Bruker	Room Room	370 ABDE 370 CF, Room 351 CF		Waters	Grand Ballroom DEF
Covaris	Room	360 CF			
Evosep	Room	310 BC			
Mass Tech Inc.	Room	342 DE			
Matrix Science	Room	351 ABDE			
NIST	Room	371 ABDE			
SCIEX	Room	360 ABDE			
Shimadzu	Room	320 BC			
Thermo Fisher Scientific	Room	361 CF			
Waters	Room	310 A			
TUESDAY, JUNE 6 / All breakfasts begin at 7:00 AM					
George R. Brown	Convei	ntion Center		Hilton	Americas
Agilent	Room	320 A		Agilent	Americas Ballroom EF
Bruker	Room	370 ABDE		MOBILion Systems	Room 335 A
Braker	Room	370 CF		SCIEX	Grand Ballroom JKL
Covaris	Room	360 CF		Shimadzu	Grand Ballroom GHI
Phenomenex	Room	361 ABDE		Thermo Fisher Scientific	Grand Ballroom ABC
SCIEX	Room	360 ABDE		Waters	Grand Ballroom DEF
Seer	Room	342 DE			
Shimadzu	Room	320 BC			
Thermo Fisher Scientific	Room	361 CF			
Waters	Room	310 A			
W		SDAY, JUNE 7 / AI	l bre	eakfasts begin at 7:00 Al	И
George R. Brown	Convei	ntion Center		Hilton	Americas
Agilent	Room	320 A		Agilent	Americas Ballroom EF
Bruker	Room	370 ABDE		SCIEX	Grand Ballroom JKL
SCIEX	Room	360 ABDE		Shimadzu	Grand Ballroom GHI
Shimadzu Room 320 BC			Thermo Fisher Scientific	Grand Ballroom ABC	
Thermo Fisher Scientific	Thorma Eigher Scientifie Deam 264 CE			Waters	Grand Ballroom DEF
Metero					
vvalerS	Room	JIUA			
7	THURS	DAY, JUNE 8 / All	brea	kfasts begin at 7:00 AM	
		George R. Brown	Con	vention Center	
SCIEX		Room 360 ABDE			
Shimadzu		Room 320 A			
Thermo Fisher Scientific		Room 361 CF, Room	371 A	ABDE, Room 371 CF	

ASMS CORPORATE MEMBERS



Corporate Member	Exhibit Booth No. Corporate Poster	Hospitality Suite at Hilton Americas	Breakfast Seminar at Convention Center or Hilton Americas
25th International Mass Spectrometry Conf.	725		
908 Devices	603		Breakfast Seminar(s), see page 16
A Chemtek Inc	215		
ACAD	918		
ACD/Labs	809		Breakfast Seminar(s), see page 16
ACS Publications	602		
Advanced Electrophoresis Solutions Ltd.	212		
Advanced Materials Technology	220		
	612		
AffiDro	621		
	600	Americas Ballroom EE	Breakfast Seminar(s), see page 16
	619		Dreaklast Seminar(s), see page 10
Alternative Biomedical Solutions	906		
AmberGen	820		
Analytical Sales and Services Inc.	506		
ANCORP	525		
Antec Scientific	413		
Ardara Technologies L.P.	CP 01		
ASI Chemicals	521		
Aspect Analytics	624		
Avanti Polar Lipids. Inc.	223		
BaySpec, Inc.	318		
BGI Americas Corporation	808		
Biocrates Life Sciences AG	519		
Biognosys	819		Breakfast Seminar(s), see page 16
Bioinformatics Solutions Inc.	812		
Biosynth	103		
Biotage	419		
Biotech Support Group	208		
Breath Explor	206		
Bright Giant	402		
Bruker Daltonics	826	Americas Ballroom AB	Breakfast Seminar(s), see page 16
Calibra Diagnostics Co., Ltd.	101		
Cambridge Isotope Laboratories, Inc.	802		
Capitainer	123		
Cayman Chemical Company	303		
CDS Analytical, LLC	514		
Cedars-Sinai Precision Biomarker	CP 02		
Cellenion	301		
Cerno Bioscience	427		
Chem Quant Analytical Solutions	523		
Chemyx	109		
CMP Scientific Corp	308		
CoAnn Technologies	721		
Computype	422		
Conquer Scientific	314		
CovalX	908		
Covaris	818	Americas Ballroom C	Breakfast Seminar(s), see page 16
CTC Analytics AG	507		
Discovery Life Sciences	CP 03		
Drug Discovery News	125		
Easymass	320		
Ebara Technologies	825		
Edwards Vacuum	209		
El-Mul Technologies	414		
Emerald Cloud Lab	425		
Entech Instruments	221		
ePrep	620		
ESI Source Solutions	326		
Evosep	/12	Room 335B	Breakfast Seminar(s), see page 16
rasmatech	107		

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Corporate Member	Exhibit Booth No. Corporate Poster	Hospitality Suite at Hilton Americas	Breakfast Seminar at Convention Center or Hilton Americas
Fossil Ion Technology	115		
Genedata	715		
GenNext Technologies, Inc.	515		
Genovis Inc	409		
GERSTEL. Inc.	309		
Hamamatsu Corporation	920		
Hamilton Company	502		
HP. Inc. Life Science Solutions	319		
HTX Technologies. LLC	508		
IDEX Health & Science	824		
IMCS	406		
IMI Adaptas	307		
Imtakt USA	803		
International Ceramic Engineering	420		
International Equipment Trading Ltd	203		
Ion Opticks Ptv I td	727		
IonBench	718		
IONICON	426		
Ionontika I td	814		
IROA Technologies LLC	501		
	607	Room 340 AB	
IPT Pentide Technologies Inc	924		
Knauer Wissenschaftliche Gerate GmbH	121		
Lab Toob Support	714		
	714		
	225		
Lood Melecular Design	724		
	612		
	013	Boom 222	
	401	Room 333	
	520		
LINI SWISSGAS	412		
Mac-MOD Analytical	515		
	527		Drackfoot Cominar(a) and name 16
Mass rech Inc.	027		Breaklast Seminar(s), see page 16
MathSpec, Inc.	CP 04		
Matavada Presisian Inc	720		Breaklast Seminar(s), see page 16
Matsusada Precision Inc	524		
Mestrelab Research	113		
MetaSci Inc.	200		
Mitewi Krawladaa kalvata Qa Ital	926		
Mitsul Knowledge Industry Co., Ltd.	227	Dears 225 A	
MOBILION Systems, Inc.	801	R00m 335 A	Breakfast Seminar(s), see page 16
Moeller Medical GmbH	520		
MPF Products Inc	325		
	914		
	408		
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	222		
	900		
	418		
	119		
	713		Breakfast Seminar(s), see page 16
	322		
NXI Power	512		
Olink Proteomics	213		
Omics Informatics	327		
Optimize Technologies	601		
Parker Hannifin	313		
Peak Scientific	518	Americas Ballroom D	
PerkinElmer, Inc.	403		
Pfeiffer Vacuum	503		
Phenomenex	321		Breakfast Seminar(s), see page 16

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Plasmin 036 number of the second sec	Phytronix Technologies	513		
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ASMS is grateful for the support of all Corporate Members. Technologies and services developed by these companies are vital to the ASMS community and the field of mass spectrometry.

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VICE PRESIDENT FOR PROGRAMS



Joseph A. Loo

University of California, Los Angeles *Vice President for Programs*

STUDENT ASSISTANTS

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

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Benjamin Garcia			Jinnui ∠hang
Anthony Gies	Andrew Mahan	Da Ren	Xueyun Zheng
Chris Gill	Tytus Mak	Emma Rennie	Mowei Zhou
Mac Gilliland	Alexander Makarov	Robert Ross	

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PROGRAM OVERVIEW

SATURDAY

9:00 ам - 5:00 рм	SHORT COURSES (Badge printing for short courses is 8-9am)			
2:00 - 5:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)			
	SUNDAY			
9:00 ам - 4:30 рм	SHORT COURSES (Badge printing for short courses is 8-9am)			
10:00 ам - 8:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)			
4:00 - 4:45 pm	ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS, Hall B3			
5:00 - 5:45 рм	TUTORIAL SESSION I, Hall B3 5:00 - 5:45 pm Mass Spectrometry and Medicine Image: Session L, Hall B3 S:00 - 5:45 pm Mass Spectrometry and Medicine Image: Session L, Hall B3 S:00 - 5:45 pm Mass Spectrometry and Anti-Doping Research Image: Session L, Ballroom A S:00 - 5:45 pm Mass Spectrometry and Anti-Doping Research Image: Session L, Ballroom A Signature Session L, Ballroom A S:00 - 5:45 pm Mass Spectrometry and Anti-Doping Research Image: Session L, Ballroom A Signature Session L, Ballroom A Signat Ses			
5:45 - 6:30 рм	Special Keynore Session, Hall B3 Image: Special Keynore S			
6:45 - 7:45 рм	CONFERENCE OPENING PLENARY, Hall A Welcome, Joseph A. Loo, University of California, Los Angeles ASMS Vice President for Programs 7:00 - 7:45 pm From Human Genome Project to Precision Medicine - A Journey in Chemistry and Technology Richard A. Gibbs			

 7:45 - 9:00 PM
 Welcome Reception, Posters-Exhibits Hall (Level One)

 Join us to celebrate the conference opening, visit exhibit booths. The Undergraduate Student Poster

 Competition is conducted during the reception. Competition posters are displayed beginning on poster board 001.

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Baylor College of Medicine

Consult online planner or mobile app for detailed program.



7:00 АМ	CORPORATE BREAKFAST SEMINARS, Convention Center (Level Three) and Hilton Americas
7:30 ам - 5:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)
8:30 - 10:30 AM	ORAL SESSIONS MOA am: Top Down Protein Analysis, Hall B3 MOB am: Imaging: Instrumentation & Method Development, Ballroom A MOC am: Clinical Analysis: Innovations, Ballroom B MOD am: Small Molecules: Structural Characterization and Quantitation, Ballroom C MOE am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, Room 332 MOF am: Covalent Labeling and Chemical Crosslinking, General Assembly A MOG am: Polymers, General Assembly B MOH am: Informatics: Metabolomics and Lipidomics, General Assembly C
10:30 am - 2:30 pm	Poster Session and Exhibits, Monday Posters, Halls BC Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm 11:30 am - 1:00 pm: Undergraduate students look for reserved tables and free lunch vouchers to Meet the Experts
2:30 - 4:30 рм	ORAL SESSIONS MOA pm: Single Cell Omics, Hall B3 MOB pm: Ion Mobility: Instrumentation & Method Development, Ballroom A MOC pm: Structural Biology, Ballroom B MOD pm: Data-Independent Acquisition and Multiplexing: Lipidomics and Metabolomics, Ballroom C MOE pm: Food Safety & Chemistry: Innovations, Room 332 MOF pm: Cancer Research, General Assembly A MOG pm: Fundamentals: Unconventional Approaches in MS, General Assembly B MOH pm: High Throughput MS, General Assembly C
4:45 - 5:30 рм	Award Lecture, Hall B3 John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry preceded by Al Yergey MS Scientist Awards Presentations Carol V. Robinson University of Oxford
5:45 - 7:00 рм	 WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm. O1 The Role of Mass Spectrometry in Emerging Energy Technologies Development, Room 310 A O2 Nucleic Acids Mass Spectrometry: Emerging Applications, Effective Analytical Strategies, and Characterization for Progressively Larger Nucleic Acids, Room 310 BC O3 Research and Funding Opportunities at the FDA: Mass Spectrometry for Drug Product Quality, Room 320 A O4 Global participatory efforts to characterize the biochemical composition of food: The Periodic Table of Food Initiative and The Proteomes that Feed the World, Room 320 BC O5 Single-Cell Proteomic Standardization: From Study Design to Data Analysis, Ballroom A O6 Networking for Scientists: Celebrating Women Mass Spectrometrists, Ballroom B O7 Exploring the World of Mass Spectral Libraries, Library Search Software and Their Applications , Ballroom C O8 Ion traps as reaction vessels, Room 332 O9 Career Opportunities for Chinese Students and Scholars, General Assembly A 10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute, General Assembly B 11 New Aspects in the Development and Implementation of Multi-Attribute Method (MAM), General Assembly C 12 Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal "bad data" in a omics core facility aka the "Bad data Workshop", Room 340 AB 13 Emerging Techniques for Rapid Fabrication in MS Laboratories, Room 351 ABDE 14 Cannabis & Hemp Science: The Importance of Mass Spectrometry, Room 351 ABDE 16 Exposome research: overcoming challenges to deliver answers, Room 360 CF 17 Using Casanovo for de novo peptide sequencing, Room 361 ABDE
7:00 - 8:00 рм	SPECIAL GAP HOUR RECEPTION SPONSORED BY AGILENT, Ballroom B Reception immediately following workshop <i>06 Networking for Scientists: Celebrating Women Mass</i> <i>Spectrometrists.</i> All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

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MONDAY



7:00 AM	CORPORATE BREAKFAST SEMINARS, Convention Center (Level Three) and Hilton Americas
7:30 ам - 5:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)
8:30 - 10:30 am	ORAL SESSIONS TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal), Hall B3 TOB am: Biomarkers: Quantitative Analysis, Ballroom A TOC am: Fundamentals: Native MS and Structures of Large Ions , Ballroom B TOD am: Informatics: Peptide and Protein Identification, Proteomics, Ballroom C TOE am: Exposomics, Toxicology, and Health Outcomes, Room 332 TOF am: Neurodegenerative Disease Research, General Assembly A TOG am: Drug Metabolism and Pharmacokinetics, General Assembly B TOH am: Imaging: Spatially-Resolved Omics, General Assembly C
10:30 ам - 2:30 рм	Poster Session and Exhibits, Tuesday Posters, Halls BC Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 рм	ORAL SESSIONS TOA pm: Instrumentation: High-Resolution Mass Spectrometry, Hall B3 TOB pm: Post-translational Modifications: Qualitative & Quantitative Analysis, Ballroom A TOC pm: Fundamentals: Ionization Methods, Ballroom B TOD pm: Informatics: Multiomics Integration and Applications, Ballroom C TOE pm: Plants and Natural Products, Room 332 TOF pm: Ion Mobility: Structure Determination & Applications, General Assembly A TOG pm: H/D Exchange: Innovations and Applications, General Assembly B TOH pm: Clinical Analysis: Applications, General Assembly C
4:45 - 5:30 рм	Award Lecture, Hall B3 Biemann Medal Lecture preceded by Research Award Presentations Brandon Ruotolo University of Michigan
5:45 - 7:00 рм	 WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm. O1 Open and Reproducible Data Analysis for FT-MS, Room 310 A O2 Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities, Room 310 BC O3 Constructing an Individual Development Plan (IDP), Room 320 A O4 The NIH and NSF Review and Funding Process, Room 320 BC O5 From data to biology: using -omics datasets to generate an unbiased hypothesis, Ballroom A O6 Recognizing the "A" in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists, Ballroom B O7 Data Independent Acquisition: After the Acquisition, Ballroom C O8 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy, Room 332 O9 Kahoot Trivia! LCMS (and other topics), General Assembly A 10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community?, General Assembly B 11 Native MS: new approaches to enable discovery in academia and industry, General Assembly C 12 New fragmentation methods as seen through the lens of radical ion chemistry, Room 340 AB 13 Non-target analysis (NTA): Modern tools for unknown analysis, Room 351 ABDE 14 Trans-Proteomic Pipeline: Recent Advances and Future Directions, Room 351 CF 15 Imaging MS: Isomer Differentiation in Biological Imaging, Room 360 ABDE 16 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence, Room 361 ABDE
7:00 - 8:00 рм	SPECIAL GAP HOUR RECEPTION SPONSORED BY SCIEX, Ballroom B Reception immediately following workshop 06 Recognizing the "A" in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists. All are welcome to join for networking focused on accessibility, diversity and inclusion.
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

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TUESDAY



7:00 AM	CORPORATE BREAKFAST SEMINARS, Convention Center and Hilton Americas
7:30 ам - 5:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)
8:30 - 10:30 AM	ORAL SESSIONS WOA am: Instrumentation: New Hybrid and Multimodal Approaches, Hall B3 WOB am: Biotherapeutics: Characterization and Quantitation, Ballroom A WOC am: Drug Discovery and Development: Qualitative and Quantitative Analysis, Ballroom B WOD am: Artificial Intelligence in MS Instrumentation and Applications, Ballroom C WOE am: Industry: Trace Analysis, Quality Control, and Automation, Room 332 WOF am: Lipidomics: New MS Technologies and Applications, General Assembly A WOG am: Stable Isotope Labeling: Applications, General Assembly B WOH am: Fundamentals: Ion Activation and Dissociation (Honoring Jean Futrell), General Assembly C
10:30 am - 2:30 pm	Poster Session and Exhibits, Wednesday Posters, Hall BC Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 рм	ORAL SESSIONS WOA pm: Instrumentation: Detection of High-Mass Analytes, Hall B3 WOB pm: Biomarkers: Qualitative Analysis , Ballroom A WOC pm: Metabolomics: New Technologies and Applications, Ballroom B WOD pm: Challenges in MS Analysis of Complex Mixtures, Ballroom C WOE pm: GC/MS: Instrumentation and Applications, Room 332 WOF pm: Quantitative Proteomics in Systems Biology, General Assembly A WOG pm: Fundamentals: Reactions of Gaseous and Solvated Ions, General Assembly B WOH pm: Environmental: Non-Target Analysis and Emerging Contaminants, General Assembly C
4:45 - 5:30 рм	ASMS MEETING, Hall B3. Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 рм	 WORKSHOPS There are light refreshments in the foyers, 5:30 - 5:45 pm. 01 High throughput screening mass spectrometry - current status and future landscape, Room 310 A 02 Late-Night Lightning Lectures!, Room 310 BC 03 Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory, Room 320 A 04 Biomarkers Development: How Mass Spectrometry Is Changing the Field, Room 320 BC 05 Ion Mobility Spectrometry: From Data to Structure, Ballroom A 06 MS Career Options: How to Kick Start Your Career, Ballroom B 07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided?, Ballroom C 08 Target Protein Degradation and MS-based Proteomics, Room 332 09 What are the future needs of photoionization mass spectrometry for complex mixture analysis?, General Assembly A 10 Houston, We Have a Microbiome Problem (and how the Metaproteomics Initiative aims to solve it!), General Assembly B 11 Hispanics and Latinx in Mass Spectrometry, General Assembly C 12 Polymeric materials: tackling hydrocarbon-based polymers, Room 340 AB 13 ProteomicsML: An online educational platform for machine learning in proteomics, Room 351 ABDE 14 Art, Museums, and Archaeology, Room 351 CF 15 Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions, Room 360 ABDE 16 Knowledge Share and Instrumentation Donations for Developing World Outreach, Room 360 CF
7:00 - 8:00 рм	SPECIAL GAP HOUR RECEPTION SPONSORED BY SEER, Ballroom B Reception immediately following workshop 06 MS Career Options: How to Kick Start Your Career. All are welcome to join for networking focused on career development.
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

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WEDNESDAY



7:00 AM	CORPORATE BREAKFAST SEMINARS, Convention Center		
7:30 ам - 2:00 рм	NAME BADGE PRINTING & INFORMATION, Level One Lobby (outside Hall B)		
8:30 - 10:30 am	ORAL SESSIONS ThOA am: Instrumentation: Ambient Ionization and Applications, Hall B3 ThOB am: Glycopeptides, Glycoproteins, and Glycomics (Honoring Catherine E. Costello), Ballroom A ThOC am: Metabolomics: Untargeted Profiling, Ballroom B ThOD am: Data-Independent Acquisition and Multiplexing: Proteomics, Ballroom C ThOE am: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers, Room 332 ThOF am: Protein-Ligand and Protein-Protein Interactions, General Assembly A ThOG am: Microbes and the Microbiome, General Assembly B ThOH am: Nucleic Acids and Oligonucleotides, General Assembly C		
10:30 ам - 2:30 рм	Poster Session and Exhibits, Thursday Posters, Halls BC Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm		
2:30 - 4:30 рм	ORAL SESSIONS ThOA pm: Instrumentation: Innovative Separation Approaches Coupled to MS, Hall B3 ThOB pm: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates, Ballroom A ThOC pm: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans, Ballroom B ThOD pm: Fundamentals: Ion Structures and Energetics, Ballroom C ThOE pm: Environmental: Innovative Approaches and Instrumentation, Room 332 ThOF pm: Lipidomics: Targeted and Untargeted, General Assembly A ThOG pm: Forensics: Innovations and Applications, General Assembly B ThOH pm: Informatics: Innovations, General Assembly C		
4:45 - 5:30 рм	PLENARY LECTURE, Hall B3 Image: Stephen Brusatte University of Edinburgh		
7:00 – 10:00 рм	CLOSING EVENT AT THE HOUSTON MUSEUM OF NATURAL SCIENCE		
	Advance purchase ticket is required.		
	Ticket sales CLOSE on Monday, June 5 at 12pm (noon).		
	Buy your ticket online via Online Registration portal (you can add-on to your existing conference registration). If you purchase after printing your name badge, you will need to re-print your badge.		
	Buffet dinner is included. Cash bars available. Enjoy the INCREDIBLE paleontology and gem exhibitions at the museum. Closing plenary speaker, Steve Brusatte, will attend the event and provide additional Q&A in the Morian Hall of Paleontology.		
	There is no organized transport to/from the event. Attendees with the closing event icon on their badge have round-trip light rail included. Please wear your badge in case there is ticket control. Engineers will identify your closing event icon as your paid ride. Light rail instructions are included in the app and will be emailed to all who have purchased the closing event.		
	The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030. If you do not wish to take the light rail, Uber/Lyft or taxis are available at standard rates.		

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THURSDAY



POSTER OVERVIEW

Poster Presentation Schedule

Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 - 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

MONDAY POSTERS

Set up all Monday posters 7:00 - 8:00 am

Odd-numbered posters present

10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

> Remove all Monday posters 7:00 - 8:00 pm

Art, Archaeology & Paleontology	001-009
Biomarkers: Discovery I	010-035
Biomarkers: Quantitative Analysis I	036-060
Biomolecular Structure Analysis:	
Chemical Crosslinking and	
Covalent Labeling	061-079
Cancer Research I	080-106
Clinical Analysis I	107-131
Covalent Labeling and Chemical Crosslinking I	132-150
Disease Biomarkers	151-171
Drug Discovery: Qualitative	
and Quantitative Analysis I	172-191
Epigenetic Modifications	192-201
Food Safety: General	202-230
Fundamentals: Ion Molecule, Ion/Ion,	
Ion/Electron Interactions	231-248
Fundamentals: Native MS	249-268
Glycoproteins I	269-293
High Throughput MS I	294-316
Imaging MS: Computational Methods, Software,	
and Analysis	317-335
Imaging MS: Method Development I	336-364
Informatics: Algorithms and Statistical Advances	365-392
Instrumentation: General	.393-411
Ion Mobility: FAIMS/DMS	412-420
LC/MS: Sample Preparation I	421-438
Lipids: General	439-466
MALDI: Applications	467-479
MALDI: Innovation in Instrumentation	
and Sample Preparation	480-492
Metabolomics: Clinical Applications	493-504
Metabolomics: Sample Preparation	.505-511
Microorganisms and the Microbiome	512-543
Nanoscale and Microfluidic Separations and MS	544-551
Peptidomics	552-569
Phosphopeptides and phosphoproteins	570-588
Plant Biology and Biotechnology	589-602
Protein Therapeutics: Structural Characterization	603-630
Proteins: Conformation Analysis	
and Structural Biology	631-662
Proteins: PTMs I	663-687
Proteomics: Infectious Diseases	688-701
Proteomics: Intact Proteins and Top Down Analysis	1702-721
Proteomics: Quantitative I	722-741

TUESDAY POSTERS

Set up all Tuesday posters 7:00 - 8:00 am

Odd-numbered posters present 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

> Remove all Tuesday posters 7:00 - 8:00 pm

Ambient Ionization: Fundamentals	
and Instrumentation	001-015
Antibodies & Antibody Drug Conjugates I	016-041
Artificial Intelligence in MS Instrumentation	
and Applications	042-062
Biomarkers: Discovery II	063-087
Biomarkers: Quantitative Analysis II	.088-111
Cancer Research II	.112-135
Clinical Analysis II	136-166
Covalent Labeling and Chemical Crosslinking II	167-193
Drug Discovery: Qualitative	
and Quantitative Analysis II	194-219
Environmental: General I	220-242
Food Safety & Chemistry: Foodomics, Allergens,	
Bacteria Foods and Supplements I	243-263
Fundamentals: Molecular Modeling /	
Quantum Mechanical Calculations	264-265
Fundamentals: Unconventional	201 200
Approaches in MS	266-279
Glycoproteins II	280-312
Imaging MS: Method Development II	313_330
Imaging No. Method Development I	3/0-350
Informatics: Protein ID and Quantification	360-370
Informatics: Workflow and Data Management	371-303
Instrumentation: Mini/Dertable/Fieldable MS	304 402
Instrumentation: Now Developments	J94-40Z
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III Mass Analyzers	403-410
ION WODINLY. General	419-440
LC/MS. Chromatography and Software	441-402
Metabolomics: Targeted	400 400
And Quantitative Analysis	403-490
Natural Products	497-505
Nucleic Acids and Oligonucleotides I	506-541
Peptides: Targeted and Quantitative Analysis	542-560
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Proteins: General and Membrane	577-592
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and Top Down Analysis II	653-674
Proteomics: Quantitative II	675-693
Proteomics: Tissue	694-713
Synthetic Polymers	714-725
Toxicology	726-733

Consult online planner or mobile <u>app for detailed program</u>.

POSTER OVERVIEW



Poster Presentation Schedule

Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 - 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

WEDNESDAY POSTERS

Set up all Wednesday posters 7:00 - 8:00 am

Odd-numbered posters present

10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present

10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters 7:00 - 8:00 pm

Ambient Ionization: Applications I	. 001-020
Antibodies & Antibody Drug Conjugates II	. 021-046
Biomarkers: Quantitative Analysis III	. 047-069
Cancer Research III	. 071-096
Carbohydrates	097-115
Data-Independent Acquisition I	116-135
Drug Discovery/DMPK/ADME	. 136-152
Drug and Metabolite Analysis	. 153-174
Environmental: General II	. 175-197
Extractables & Leachables	. 199-204
Forensics	. 205-231
Fundamentals: Formation and Structures	
of Big lons	. 232-233
Fundamentals: Ion Spectroscopy	. 234-241
Fundamentals: Ionic Clusters, Nanomaterials,	
and Catalysis	. 242-244
Fundamentals: Ionization	. 245-257
GC/MS: Instrumentation and Applications	. 258-280
H/D Exchange: Hardware, Software	
and Methodology	. 281-297
High Mass Accuracy/High Performance MS:	
Applications and Instrumentation	. 298-321
Imaging MS: Disease Markers	. 322-334
Imaging MS: Pharmaceuticals, Metabolites,	
Lipids, and Glycans I	. 335-355
Industry: Trace Analysis, Quality Control,	
and Automation	. 356-371
Informatics: General, SRM, and DIA	. 372-380
Informatics: Multiomics Integration	. 381-396
Instrumentation: New Concepts	. 397-406
Instrumentation: New Developments	
in Ion Detection	. 407-408
Instrumentation: New Developments in	
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Ion Mobility: Applications I	. 433-451
Ion Mobility: Fundamentals	. 452-460
Ion Mobility: Structure	. 461-482
LC/MS: General	. 483-510
Lipids: ID and Structural Analysis	511-542
Lipids: Targeted and Quantitative Analysis	. 543-568
Metabolomics: Untargeted Metabolite Profiling I	. 569-594
Neurodegenerative Disease Research I	. 595-617
Proteomics: Quantitative III	. 618-638
Single Cell MS I	. 639-661
Small Molecules: Qualitative and	
Quantitative Analysis I	. 662-681
Stable Isotope Labeling	. 682-695
Systems Biology	696-711
Viruses and Virus-Like Particles	. 712-730

THURSDAY POSTERS

Set up all Thursday posters 7:00 - 8:00 am

Odd-numbered posters present 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

> Remove all Thursday posters At 2:30 pm

Ambient Ionization: Applications II	. 001-018
Antidoping, Cannabis, and Opioid Detection	. 019-025
Data-Independent Acquisition II	. 026-046
Education: Teaching MS and Teaching with MS	. 047-052
Elemental Analysis	. 053-054
Energy: Petroleum, Biofuels, and Algae	. 055-064
Environmental: General III	. 065-089
Environmental: Pharmaceuticals and Pesticides	. 090-101
Exposomics	. 102-121
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Bacteria, Foods, and Supplements II	. 122-147
Fundamentals: Ion Activation/Dissociation	. 148-159
Fundamentals: Ion Structure/Energetics	. 160-170
Glycomics	. 1/1-191
H/D Exchange: Protein Structure/Function	. 192-227
High Throughput MS II	. 228-253
Imaging MS: Instrumentation	. 254-267
Imaging MS: Pharmaceuticals, Metabolites,	
Lipids, and Glycans II	. 268-303
Imaging: Spatially-Resolved Omics II	. 304-322
Informatics: Metabolomics and Lipidomics	. 323-356
Informatics: Peptide ID and Quantification	. 357-379
Ion Mobility: Applications II	. 380-401
Isotope Labeling and Fluxomics Applications	. 402-410
LC/MS: Sample Preparation II	411-432
Lipids: Profile Analysis	. 433-455
Metabolomics: General.	. 456-490
Metabolomics: Identification of	404 500
Unknown Metabolites	. 491-500
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Dentidee: Identification and	. 222-201
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Pragmentation Mechanisms	502-091
Prepides. PTM Identification	621 625
Process Development MS	626 655
Proteomics: Now Approaches	. 020-000
Single Coll MS II	620-000
Small Moloculos: Qualitativo	009-113
and Quantitative Analysis II	711-725
anu Quantilative Analysis II	. 1 14-130





MONDAY WORKSHOPS, 5:45 -7:00 PM

01 The Role of Mass Spectrometry in Emerging Energy Technologies Development Energy Petroleum & Biofuels Interest Group Presiding: Yuri Corilo, Leonard Nyadong Room 310A

Alternative and emerging energy technologies including batteries, hydrogen, nuclear and renewables such as solar, wind, hydropower, geothermal and biofuels all play a crucial role in the future of our planet. They provide a sustainable solution to our growing energy demands while reducing our dependence on finite resources such as oil and gas. From an economic perspective, alternative energy technologies can lead to reduced energy costs, increased energy security, and new job opportunities in the energy industry. Finally, from an industrial perspective, the development and use of emerging energies can lead to technological advancements and innovations in the energy sector, contributing to the growth of the global economy.

Mass spectrometry technology has played a key role over several decades in the development of fossil fuels and to a lesser extent, alternative energies including biofuels. Mass spectrometry allows for the precise analysis of chemical compounds, which provides the detailed molecular composition of energy feedstock materials. The information is essential for optimizing the energy source production and refining processes, leading to more efficient and cost-effective energy generation. Mass spectrometry is beginning to play a role in developing new energy technologies, such as advanced batteries and fuel cells, by enabling scientists to analyze and improve their performance properties.

This workshop will provide the opportunity to discuss the role of mass spectrometry in development of alternative energy technologies. The workshop will feature practitioners who are applying mass spectrometry in alternative energy research to discuss experiences, enablers, challenges, and the outlook of the role of mass spectrometry in emerging energy fields.

02 Nucleic Acids Mass Spectrometry: Emerging Applications, Effective Analytical Strategies, and Characterization for Progressively Larger Nucleic Acids *Oligonucleaotides and Nucleic Acids Interest Group* Presiding: Varun Gadkari, Jennifer Lippens, Robert Ross Room 310BC

Recently, nucleic acids have returned to the forefront of biomedical research, with rapidly growing interest in fundamental, translational, and pharmaceutical research areas. Scientists are seeking new and improved methods for characterizing challenging and relevant, nucleic acid targets and therapeutics, including oligonucleotides ranging in size from antisense oligonucleotides to mRNA. This interest group seeks to bring together ASMS members across multiple sectors to discuss the latest in nucleic acid mass spectrometry including sample production and preparation, method development, analysis strategies, application needs, and more. Long-term, the goal is to foster a strong community in this space and accelerate the development of mass spectrometry-based strategies for nucleic acids research.

Our 2023 format will consist of 4-5 panelists from diverse backgrounds and including both mid-to-late stage career established researchers as well as junior/early career scientists to provide exposure for emerging researchers. Panelists will present a short intro of their current research followed by a moderated open discussion/question and answer session over the presentations and any other questions that attendees may bring forward. We will also gauge interest for a future Asilomar Meeting focusing on nucleic acids through participant surveying and gather feedback on topics surrounding nucleic acid mass spectrometry that would be of interest for future ASMS workshops. We look forward to workshop participants coming with their most burning questions and to a great discussion in this exciting space.

03 Mass Spectrometry for Drug Product Quality: Research and Collaboration Opportunities Independent

Presiding: Jinhui Zhang, Mack Shih

Room 320A

The purpose of this workshop is to provide mass spectrometry researchers in academia a broader picture of the importance of mass spectrometry in drug evaluation and research, as well as protecting public health at the FDA. The workshop will start with a set of guiz/poll to check the attendees' knowledge on small and large molecule drugs discovery, development, evaluation, and the role of mass spectrometry in each of the stages. Then, we will share with the attendees several research "stories" we accomplished in the past several years as case studies to highlight how we implement advance mass spectrometry and automation tools at the FDA to: 1) address carcinogenic drug impurities to protect public health; 2) support the modernization of over-thecounter drug products; 3) enable quality surveillance of marketed drug products; 4) in-depth investigation on mass spectrometry parameters to assure data quality for pharmaceutical analysis and bioanalysis In the end, we will discuss how academic researchers can collaborate with FDA to improve drug product quality research.

04 Global participatory efforts to characterize the biochemical composition of food: The Periodic Table of Food Initiative and The Proteomes that Feed the World Independent

Presiding: Jessica Prenni, Bernhard Kuster Room 320BC

Food is at the center of addressing some of the world's most urgent challenges. However, our scientific understanding of the biochemical composition of food and the organisms that underlie it is rudimentary at best. This workshop will present two global efforts focused on improving our understanding of what is in our food. (1) The Periodic Table of Food Initiative (PTFI) is developing standardized, fully democratized LC-MS based technology platforms for generating comprehensive food composition data. These platforms are open-source and can be used by laboratories around the world to populate a reference database that enables open access and comparability of foodomics data. (2) The Proteomes that Feed the World (PFW) is mapping the proteomes of all major tissues and organs of the 100 crop plants most important for human nutrition. This effort will create a Crop Proteome Atlas of high value to academia as well as the agricultural and food industries. The objectives of this workshop will be to: (1) introduce the PTFI and the PFW to the broader mass spectrometry community; (2) provide updates on progress as well as spark innovative ideas and feedback and (3) discover new opportunities for engagement.



MONDAY WORKSHOPS, 5:45 -7:00 PM

05 Single-Cell Proteomic Standardization: From Study Design to Data Analysis Independent

Presiding: Jennifer Van Eyk, Peter Nemes Ballroom A

Recent advances in mass spectrometry technology have extended proteomics into single cells. A rapidly growing number of laboratories seek to adapt single-cell mass spectrometry across a broad swath of biology. Technologies based on automated sample preparation, liquid chromatography and capillary electrophoresis as well as mass spectrometry have enabled ultra-high sensitive quantification of hundreds-to-thousands of proteins in various cell types. These studies are revealing previously unknown (and unexpected) paradyms about the molecular organization of the cell. Yet there are many challenges associated with the design, execution and data analysis of singlecell proteomics. To facilitate scientific rigor and reproducibility, we propose a single-cell proteomics workshop. This workshop will fulfill the following aims: (1) Update the scientific community of technological advances with a focus on study design, execution, and data analysis; (2) disseminate single-cell methods and protocols to promote technological adaptation with a focus on recent community-wide standards established in single-cell mass spectrometry proteomics; (3) identify remaining challenges in single-cell proteomics; (4) recruit new members to the field. The workshop will focus on challeanges and solutions. It will start with each panelist giving a 5 min talk overview of their biggest challeange and solutions and end with a roundtable discussion of panelists, who will solicit and answer questions from attendees. Moderator, Jennifer Van Eyk. Panelists: Nikolai Slavov (Northeastern U.) - Study design and Standards; Lingjun Li (U. of Wisconsin) - Sample prep; Ryan Kelly (Brigham Young Unv) sample intergration with MS; Peter Nemes (U. of Maryland) - MS throughput; Fabio Gomes (Scripps) - Topdown SCP; Olga Vitek (Northeastern Univ) - Statistics with respect to SCP.

06 Networking for Scientists: Celebrating Women Mass Spectrometrists Independent

Presiding: Stacy Malaker, Aivett Bilbao, Julie Courraud Ballroom B

This year we plan on having a more interactive networking event. To begin, as in years past, 3-4 new panelists will be introduced and then take time to discuss career paths they have followed, what factors they considered when making big decisions, and advice they would give to a woman and members from underrepresented minorities facing the same challenges. Then, we will ask the attendees to answer questions via Kahoot (or similar polling application), which the panelists will then comment on and discuss. The goal here would be for the participants to see they are not alone in their experiences and/or challenges. Some example questions for this event could include:

- Has there been a time you felt seen and supported as a woman in your field?
- Do you feel like you have a positive network/support system at work or your program?
- Do you have a mentor you can look up to or help you navigate career challenges?
- Have you looked for networking experiences with other women in STEM?

Have you seen improvements to promote gender equality and diversity inclusion within your team/group?

Following this, a larger cohort of organizers/volunteers (approximately 15-20) of varying backgrounds and career stages will then lead small group discussions. The attendees will be encouraged to join a group, share their experiences and contact information, then network accordingly. The small group discussions will last for the remainder of the workshop before the gap hour networking sponsored by Agilent.

07 Exploring the World of Mass Spectral Libraries, Library Search Software and Their Applications Mass Spectral Libraries Interest Group

Presiding: Emma Rennie, Xiaoyu Yang, Melinda McFarland Ballroom C

The growing amount of data produced by mass spectrometry has made the identification of compounds in routine data analysis increasingly challenging. The use of mass spectral (MS) libraries has emerged as a valuable solution for fast and accurate compound identification. This workshop delves into the most recent advancements in MS libraries, exploring their use, application, and accompanying software tools. A panel of leading experts will present on the current state of MS libraries and the software tools they have developed or utilized in their work. They will also provide their perspectives and insights on the development and application of MS libraries. Following their presentations, there will be an opportunity for a brief Q&A session, followed by an interactive discussion on a range of topics, such as: the available MS libraries; library search software; integration with open source software platforms (e.g. Skyline and GNPS); AI applications; data processing software for searching and library building; and the use of libraries in areas such as metabolomics, food science, clinical proteomics, and environmental analysis. By the end of the workshop, participants will have a comprehensive understanding of how MS libraries can enhance their data analysis and the wide variety of software tools that can support this process.

Panelists: Michael MacCoss (University of Washington), Stephen Stein (NIST), Lloyd Sumner (University of Missouri), Arpana Vaniya (UC Davis), Mingxun Wang (UC Riverside).

08 Ion traps as reaction vessels Ion Trap MS Interest Group Presiding: Dalton Snyder, Lucas Szalwinski

Room 332

Ion traps are remarkably versatile analytical devices. They are capable of a wide range of capabilities that other analyzers can only dream of, from ion isolation to mass analysis and a full suite of MS/MS experiments. But that's not all! Ion traps can also serve as clean, selective, fast, and efficient reaction vessels for squeezing every ounce of chemical and structural information out of analytes.

This year's Ion Trap MS workshop will focus on the ion trap's ability to serve as a vessel for conducting ion/ion, ion/molecule, ion/photon, and fragmentation reactions. A diverse selection of speakers from academia and industry will give lightning talks on reactions of all sorts. These talks will then be followed by a panel discussion with audience Q & A.





MONDAY WORKSHOPS, 5:45 -7:00 PM

09 Career Opportunities for Chinese Students and Scholars Independent

Presiding: Junmin Peng, Shuguang Ma General Assembly A

With the rapid development of mass spectrometry technologies and the increasing applications to academic research, medicine, industry, and regulatory agencies, a growing number of mass spectrometrists including thousands of Chinese students and scholars are trained. The workshop for Career Development Opportunities for Chinese Students and Scholars aims to provide career perspectives to students and scholars to learn the career paths at different career stages. We will invite four speakers from academia, clinic, industry, and regulatory agencies to share their experiences for career development. We will also assemble a group of discussion panelists to answer questions from the audience. We believe the workshop is beneficial to both students and scholars of all ASMS members and potential employers. The workshop will provide opportunities for students and scholars to prepare for their career development during and after mass spectrometry training and help them to set up career goals in the field of mass spectrometry.

10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute *Top-Down Proteomics Interest Group* Presiding: Yuri van der Burgt, Mowei Zhou

General Assembly B

Top-down mass spectrometry (TDMS) provides unique and complementary information at the intact protein level that is commonly masked when using bottom-up proteomic methods. Nevertheless, the community has experienced various challenges in adopting TDMS strategies due to a lack of a "one size fits all" solution. The difficulty is exacerbated by many options for sample preparation protocols, instrument parameters, and data analysis software, especially when dealing with complex samples. After the feedback from the 2022 workshop, the Consortium for Top-down Proteomics (CTDP) has established an Early Career Researcher (ECR) committee to help identify opportunities and plan activities to address many of these challenges as a community.

In this workshop, we will first have ECR representatives: 1) present planned near-term activities about more expertise sharing, including experimental protocols; 2) discuss the vision for the newly opened CTDP LinkedIn group for barrier-free communication; 3) discuss an initiative to create "golden datasets" for software development with inputs from the community; 4) solicit ideas for further improvements and new activities. This will be followed by an update about the CTDP initiative on an interlab study of capillary electrophoresis from Alexander Ivanov, Liangliang Sun, and Kevin Jooss. Last, we will host an open panel discussion for the audience to ask questions and suggest ideas.

Lastly, we will invite two newcomers to the field to discuss future TDMS applications with the audience, with the goal of inspiring new ideas and collaborations.

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11 New Aspects in the Development and Implementation of Multi-Attribute Method (MAM)

Biotherapeutics Interest Group Presiding: Da Ren, Andrew Mahan General Assembly C

The advances of new indication and therapeutic modalities in the pharmaceutical industry drives the development of new analytical methods that provide enhanced content in a more efficient manner. In the past of decade, liquid chromatography (LC)-mass spectrometry (MS)-based Multi-Attribute Method (MAM) has successfully demonstrated its capability in replacing traditional chromatographic, electrophoretic, and binding assays for monitoring both product and process quality attributes (Rogers R. et al., AAPS J, 2017, Ren D., Trends Biotechnol. 2020).

As we enter a new decade of technology and method development, MAM's utility is expanding. Recent advances in mass spectrometry instrumentation have provided novel opportunities in reforming the original MAM. The industry-wide MAM Consortium inspires method development and diversity for new MAM approaches that are fitting into different application in biopharma R&D schemes. New approaches to MAM are emerging, e.g. fully automatic sample preparation, MAM for cell and gene therapies, compact MS for MAM in QC, and new data acquiring approaches. The biotherapeutic interest group workshop offers a forum for members to share and discuss those new aspects in the development and implementation of MAM.

12 Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal "bad data" in a omics core facility aka the "Bad data Workshop" *Analytical Lab Managers Interest Group* Presiding: Brett Phinney, Uri Keshet, Dave Quilici

Room 340AB

Bad samples, bad data? Data quality in the omics core lab is a challenging task because of the large-scale and untargeted nature of omics experiments, and the variety of instruments and assays that a core lab is expected to provide. Some of the causes for bad data are Sub optimal sample prep , miss behaving LC's, and Mass spectrometers on the verge of blowing up. While there are ways to minimize bad data, it still happens, and it happens more than we like. Come to the workshop and share tips and strategies for preventing and, if necessary, dealing with bad data in both proteomics and metabolomics core facilities. After a few brief examples from our speakers, audience members will be given a shoulder to cry on or asked to share their strategies for dealing with BAD DATA

13 Emerging Techniques for Rapid Fabrication in MS Laboratories Independent Presiding: John F. Cahill, Vilmos Kertesz

Room 351ABDE

The use of additive and subtractive manufacturing, as well as open-source electronic prototyping platforms, has become increasingly prevalent in scientific research, including in the field of MS. These technologies allow for rapid prototyping of components and devices, which can greatly enhance the efficiency of the research process. In the workshop series, participants will share their experiences with designing and fabricating custom components. We will also discuss the use of open-source



MONDAY WORKSHOPS, 5:45 -7:00 PM

electronic prototyping platforms such as Arduino or Raspberry Pi to develop custom electronics for instrument control and data acquisition. Participants can share best practices and their best 'tips and tricks' for designing and prototyping components quickly and efficiently. Overall, the workshop series will be a valuable opportunity for MS researchers to share knowledge and expertise related to the use of these auxiliary technologies, with the goal of advancing research in the MS field.

14 Cannabis & Hemp Science: The Importance of Mass Spectrometry Independent Presiding: Jordan Witkop Room 351CF

The global legalization of cannabis and hemp-derived medicine and consumer products has paved the way for advances in cannabis science from the accurate detection of active cannabinoids and harmful, trace contaminants to more informative strain typing, advanced breeding programs and clinical research. GOALS: Deliver key opinion leader panel discussions on novel applications of cannabis and hemp in the medical arena as well as future directions. Foster discussions regarding the applications of mass spectrometry to cannabis and hemp science and research. Encourage expanded use of mass spectrometry in cannabis/ hemp applications by sharing information and discussing emerging growth areas.

Panelists:

- Brett Ginsburg, PhD (START Center Genetic Research Professorship Department of Psychiatry, The University of Texas Health Science Center at San Antonio) "Using Mass Spec to evaluate recreational and medical cannabinoid use in clinical samples."
- Russell W. Jessup, PhD (Associate Professor of Perennial Grass & Industrial Hemp Breeding Department of Soil and Crop Sciences, Texas A&M University) "Developing highthroughput & low-cost chemotyping tools"
- Matt Vergne, PhD (Associate Professor, Dept of Pharmaceutical Science, Lipscomb University) "Development of a cannabinoid testing method using blood plasma collection cards and LC-MS/MS"

15 Mind the (Translation) Gap Clinical Chemistry Interest Group Presiding: Brian Rappold Room 360ABDE

The ASMS annual meeting is replete with novel technologies, new biomarkers and evolving means to assess diseases in patients. However, the path to utilize these innovations in the clinical environment is not a common point of discussion. This workshop will discuss the framework of translating an innovation into reality with a panel of experts in diagnostic medicine, including representatives from manufacturers of FDA-approved materials and assays, venture capital/biotech investment and international reference labs. A discussion of the regulatory and financial environment will take place with a "Shark Tank"-like approach; imaginary proposals will be offered to the panel to launch a conversation about bridging the gap from a discovery to a deployment in a diagnostic laboratory.

16 Exposome research: overcoming challenges to deliver answers

Exposomics Interest Group Presiding: Benedikt Warth, Ruth Marfil-Vega, Silvia Balbo

Room 360CF

The workshop will inform and discuss the latest developments in the expanding field of exposome research. An overview of the latest technological developments and global initiatives will be presented.

The discussion will focus on the tools, infrastructure, and support necessary to continue successful exposomics research. This includes comprehensive mass spectrometric and bioinformatic workflows. Researchers from renowned labs working in the area will be present to share their views on current shortcomings (infrastructure, standardization, harmonization, chemical coverage, sensitivity issues) but also share their vision of how true omic-scale exposure assessment can be successfully established. Future directions of exposomics will be discussed in light of a massive push coming from both, US-based and European initiatives leading the way toward innovative research in the arena of environmental health and public and personalized prevention.

17 Using Casanovo for de novo peptide sequencing Independent

Presiding: Melih Yilmaz, William Noble, Will Fondrie Room 361ABDE

Casanovo is a new de novo peptide sequencing method that uses a deep learning model trained on massive data to achieve very high prediction accuracy. The software is implemented in Python and is available open source with an easy installation procedure. The goal of this hands-on workshop is to train users to install the software, run Casanovo using a pre-trained trypsin or non-enzymatic model, and interpret and visualize the results. We will also show you how to fine-tune the model with data from your own lab to make Casanovo work well for you. Attendees may wish to bring their own laptops to follow along with the demos. The workshop will close with a discussion of the pros and cons of de novo sequencing, with the aim of eliciting feedback for improving the utility of Casanovo and other similar tools for the user community.





TUESDAY WORKSHOPS, 5:45 -7:00 PM

01 Open and Reproducible Data Analysis for FT-MS FTMS Interest Group Presiding: David Butcher, Yuri Corilo

Room 310A

The proposed FT-MS interest group workshop will focus on applying open and reproducible workflows to analyze FT-MS data. It will build on the designation of 2023 as the Year of Open Science by the White House Office of Science and Technology Policy. While the general subjects of open science and FAIR data will be mentioned, the workshop's primary focus will be practical methods that researchers can use to ensure that the analysis of data collected using FT-MS instruments can be effectively shared and reproduced by other researchers. This will include using computational workflows implemented in opensource programming languages such as Python and R, workflow languages, containerization technologies, metadata capture and standards, and other existing and emerging methods. The exact content of the workshop will be at the discretion of the speakers, who will have expertise in software and workflow development for FT-MS data analysis.

The workshop will consist of a 15-minute introduction given by the co-chairs, followed by three 10-minute talks/demonstrations given by the recruited speakers on a specific aspect or example of reproducible analysis of FT-MS data. In the final 30 minutes, guestions will be taken from the audience.

The overall goals are to:

- 1. Provide researchers with experience in computer programming and practical advice in making their data analyses open and reproducible.
- Communicate to researchers without computer programming skills the value gained from implementing reproducible data analysis practices.
- 3. Promote the use of these practices in the FT-MS community.

02 Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities DMPK Interest Group Presiding: Lina Luo, Holly Maw Room 310BC

The human radiolabeled adsorption-distribution-metabolismexcretion (ADME) study provides a quantitative and comprehensive overall picture of the disposition of a drug and is required for new drug approval. The accelerator mass spectrometry (AMS), which enables microtracer and microdosing studies, to ultrasensitively quantify radiolabeled compounds in biological matrices, offers various strategic advantages in drug development. Advanced AMS technology allows administration of 100-fold to 1000-fold lower amounts of carbon-14, which significantly reduces radiation burden to human volunteers. With microtracer hADME studies, the safety of trial participants is greatly improved as well as the need for a GMP grade drug substance can be eliminated. This is especially critical in vulnerable populations, such as pediatric or pregnant subjects, which further reenforce the need to keep radiation burden to a minimal level. AMS further facilitates innovative approaches for study designs to allow dosing by alternative dose routes. Administration of drug via routes such as ocular and dermal can be introduced with the sensitivity of AMS. With the AMS-enabled ADME study, we can have data on a complete metabolic profile in circulation and excreta earlier than

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the currently well-established timeline (before end of Phase II). Overall, the drug development timeline can be accelerated with the AMS-enabled ADME study, and a complete understanding of drug disposition can be achieved earlier. This workshop will bring together established researchers from the pharma industry and research institution to discuss current utility and future opportunities of the AMS technology in drug development.

03 Constructing an Individual Development Plan (IDP) Career Development Interest Group Presiding: Troy Wood

Room 320A

The concept of the Individual Development Plan (IDP) is employed frequently in industrial settings to help employees construct a definitive plan for achieving career goals; however, IDP can be used in any work setting. I(n 2003, the Federation of American Societies for Experimental Biology (FASEB) proposed an IDP framework for postdoctoral fellows; subsequent polling of postdocs who developed an IDP reported it helpful to self-assess their abilities and skills, and identify which skills they would need for career advancement. Borrowing this framework, we will provide an overview of developing an IDP: 1) self-evaluation of skills, interests, and values, 2) use the self-assessment as a guide to evaluate and explore career opportunities (including alternative options), 3) setting specific goals for the aspired-to career path, including discussion with mentors, and 4) putting the IDP into place. We hope the workshop will either lead to the formulation of individual IDP or will refresh thoughts to those with existing IDPs. Although geared toward young mass spectrometrists, members from any stage of their career are welcome.

04 The NIH and NSF Review and Funding Process Independent

Presiding: Salvatore Sechi, Kelsey Cook, Douglas Sheeley, Kenneth Ryan

Room 320BC

Many ASMS members and conference participants are supported by the National Institutes of Health and 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. Tips on grant writing and insights into the review process will be presented. The session will also provide an opportunity to inquire about the latest NIH and NSF initiatives and priorities. 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.

05 From data to biology: using -omics datasets to generate an unbiased hypothesis Bioinformatics MS Interest Group

Presiding: Katarzyna Kulej, Claire O'Donovan Ballroom A

This workshop will discuss the common practices to "break the ice" in data simplification and interpretation. Most ASMS conference attendees deal with large datasets that require processing, sorting,



TUESDAY WORKSHOPS, 5:45 -7:00 PM

filtering, and representation. Is there a rulebook for approaching these tables? The answer is no. However, we will discuss some of the most used and accepted workflows for interpreting an -omics dataset and how best to approach data representation. We will focus on both understanding the quality of MS-data output and reducing the complexity of biological data extracted. At the end of this session, we expect attendees to have acquired tips and tricks to minimize the activation barrier facing -omics data interpretation.

We will present some of the most commonly used and freely available software to interpret proteomic data and display data graphically. We will focus on how to analyze proteomes, including their protein post-translational modification (PTM), without needing a driving hypothesis. Furthermore, we will introduce the repositories used to match newly generated data with preexisting knowledge on gene/protein/PTM biodata and how to cross-validate novel findings with what is reported in the literature. Finally, we will open a roundtable discussion of the most common issues and bottlenecks in data interpretation. We will welcome different perspectives, ideas, and practices in unbiased hypothesis generation using -omics datasets. Ultimately, our overall goal is to encourage non-experts in bioinformatics to explore user-friendly resources for MS data analysis.

06 Recognizing the "A" in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists Membership, Diversity, and Inclusion Committee Presiding: ASMS Membership, Diversity, and Inclusion Committee Members Ballroom B

Accommodations for persons with disabilities are rarely implemented with a "one-size fits all approach" as disabilities can be multi-faceted, range in severity, vary in impact based on the setting, and be classified as visible or non-visible in nature. Accessibility barriers, especially those experienced in a laboratory or workplace environment, can stifle knowledge exchanges, limit collaboration and participation, or reduce a scientist's quality of life. It is therefore important to promote a work culture where every member is appreciated, respected, and given the tools to succeed. Dialogue is the first step in recognizing the needs of persons with disabilities and formulating effective accommodation ideas.

The ASMS Membership, Diversity, and Inclusion (MDI) committee will host the first ASMS workshop on accessibility. To address the needs of visible and non-visible disabilities, the workshop program will be divided into 3 segments that highlight physical, sensory, and cognitive disabilities. The workshop format will feature a panel composed of students, post-docs, faculty, and staff that will speak to the unique issues experienced by persons with disabilities as well as evidence-based solutions that have been implemented to make laboratories and work environments more accessible.

07 Data Independent Acquisition: After the Acquisition Data Independent Acquisition Interest Group Presiding: Lindsay Pino, Lukas Reiter Ballroom C

Data independent acquisition (DIA) has drawn the interest of (prote)omics researchers thanks to its high levels of reproducibility, capacity for large sample sizes, and the completeness of quantitative data. As academia and industry strives towards scaling workflows to hundreds or thousands of samples, derived

from single cells, cell line screens, or large clinical cohorts, the boundaries of throughput and proteome depth are rapidly increasing, requiring advances in liquid chromatography-mass spectrometry systems and bioinformatics to support the scope of experimentation.

In this workshop, we invite experts in the field to discuss topics of importance and debate amongst DIA users. We explore both fads and trends that are emerging as DIA opens proteomics to larger and larger data, with a focus on what happens after acquisition, from preliminary data processing to data storage to formatting and data interpretation and dissemination. This includes the use of deep learning to better process DIA on the level of spectra but also on the level of interpreting large scale sample cohorts. Further, we are going to discuss how the next 10 years of DIA may look like or what users would like to see developed in the next 10 years. Along these lines, we'll revisit some of the topics from previous DIA workshops to compare the direction the field seemed to be going to where things ended up going. For example, the prediction last year was that "more peptide/protein detections" would be this year's great breakthrough, stemming from increased use of AI/ML in data analysis. We will also explore new applications for DIA, or the lack of new applications, to evaluate where DIA is being most heavily used versus applications that are still challenging for DIA approaches.

08 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy Metabolomics Interest Group

Presiding: Tytus Mak, Thomas Horvath, Maryam Goudarzi Room 332

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As of January 2023, all National Institutes of Health (NIH) funded investigators are required to abide by the new NIH Data Management and Sharing Policy (DMS). This policy requires new proposals to include a data management plan, and experimental data generated using NIH funds to be Findable, Accessible, Interoperable, and Reproducible, or FAIR. FAIR data sharing is integral to spur research reproducibility, promote data reuse, and accelerate research. The meeting will open with a few opening remarks regarding the theme of the meeting, a short introduction for each of the speakers, and a short Slido poll regarding the challenges facing the community and suggestions for the ASMS 2024 meeting topic (5-10 mins). The first speaker will be Dr. Reed Shabman, Program Officer at NIH-NIAID (or another NIH representative), who will comment on the implementation of the new DMS policy (15 mins). Then, a short presentation (15 mins) on the advantages, obstacles, and solutions of FAIR Data Sharing in scientific research will be presented by Dr. Laura Hughes (Scripps Research). Then, attendees will be asked to form small groups to discuss the obstacles and potential solutions for complying with the DMS policy in their respective laboratory environments (20 mins). The balance of the time will be spent discussing the findings discussed in each of the small group interactions (~15-20 mins).

09 Kahoot Trivia! LCMS (and other topics) LCMS & Related Topics Interest Group

Presiding: James Dodds, Jack Ryan, Karen Butler General Assembly A

For the past couple of years we've been hosting a phone based trivia evening where attendees can login to a free app (Kahoot) and play along with trivia questions against their friends for



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enjoyment and the top 3 players get prizes (usually stuffed animals like microbes and such).

Our attendance last year was something like 80 people, not sure how that stacks up to the other workshops. Maybe it was Monday/ Tuesday night, can't recall.

10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community? *Lipids & Lipodomics Interest Group* Presiding: Michal Holcapek, Jeffrey McDonald

General Assembly B

The lipidomics community is growing, and many newcomers are joining or at least using the lipidomics data in their research. However, there are not yet standardized methods for lipidomic analyses and data reporting, which may sometimes lead to confusion. The International Lipidomics Society (ILS) was established in 2019 with the goal of fostering the cooperation of lipidomic researchers and harmonizing methodologies, nomenclature, data reporting, and organization of ring trials. This lipidomics workshop has two main objectives. First, we would like to introduce the key activities of the ILS, such as the harmonization of lipidomics workflows with the help of minimum reporting standards, the updated shorthand lipid nomenclature, and the organization of ring trials. Second, we would like to initiate a discussion with the attendees to get a feeling of what the lipidomics community would expect from ILS and where ILS still has room for improvement. This discussion can also be regarded as an incentive for the lipidomics community to get involved in ILS and actively shape the future of the research field of lipidomics.

Workshop schedule (75 min)

- M. Holčapek Introduction & CLIG human plasma lipidome trial (15 min)
- \ddot{i} A. Gassiot Ceramide and bile acids ring trials (15 min)
- i J. McDonald Minimum reporting checklist (15 min)
- i Discussion (30 min) What else can we do for lipidomic community? Suggestions and ideas on how we should do together a better job for the lipidomic community.

11 Native MS: new approaches to enable discovery in academia and industry Native Mass Spectrometry Interest Group

Presiding: Justin Benesch, Kristine Parson, Art Laganowsky General Assembly C

Native MS is recognized as a cutting-edge approach in the molecular characterization of protein targets and therapeutics, and their interactions. It can provide information on assembly stoichiometry, structural integrity, ligand and drug binding, all with unrivalled mass resolution and accuracy. As research targets in academia and industry become more challenging, there is an increasing need to push the limits of native MS in terms of the samples it can address, the ease in which it does so, and how it can integrate with orthogonal technologies.

We are witnessing a continuing growth in native MS and associated methodologies. Exciting developments have been made in the ability to deliver samples of greater inherent complexity, and from "dirty" sources, as well as big steps forward in online delivery and throughput. At the same time, there is continued effort at the interfaces with other MS-based or structural biology methods.

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This workshop will highlight the cutting edge of native MS technology development, focusing on disseminating the newest approaches in the field that are breaking down barriers for examining previously intractably complex samples. This workshop, in an informal style, will therefore demystify the state-of-the-art, and be valuable both for newcomers to the individual topics as well as those already proficient in the native MS field.

The native MS workshop has long supported collaboration and knowledge transfer between academia and industry. We are assembling a diverse panel of experts from both theatres; they will each deliver short presentations, and (together with the attendees) participate in an open discussion facilitated by the workshop organisers.

12 New fragmentation methods as seen through the lens of radical ion chemistry

Fundamentals Interest Group Presiding: Yury Tsybin, Alexander Makarov, Room 340AB

Rapid advances in the resolution and sensitivity of mass spectrometry instrumentation over the last decade have fueled the steady performance enhancement of the arsenal of diverse fragmentation methods. In addition, novel and old ion activation and dissociation reaction ideas have been probed experimentally to further increase the MS/MS capabilities. The most notable recent advances relate to the broader use of higher-energy electrons in, e.g., EID (or EIEIO?) for singly charged small molecule analysis and the combination of multiple fragmentation methods for better characterization of macromolecular complexes.

The dramatic expansion of available data raises the question of whether the established understanding of underlying gas phase ion activation and dissociation chemistry needs any revision - or whether we are already well equipped with our existing models. This interactive workshop will involve speakers from diverse

research areas united by the passion for gas phase radical (and non-radical) ion chemistry and its use to advance the frontiers of analytical science.

They all probably would endorse (and suggest their versions of) the poem composed on the radical ion chemistry theme by ChatGPT:

Radical ions, charged and free, Soaring high with energy, In mass spectrometry they dance, A chemical romance. With a radical push. They're torn apart with a rush, Their masses revealed, Their secrets to be unsealed. In the hands of the expert, This tool never falls short, Unlocking the mysteries, Of the world's great histories.

13 Non-target analysis (NTA): Modern tools for unknown analysis Environmental Applications Interest Group Presiding: Ahmed Hamid, Kevin Tucker

Room 351ABDE

Environmental pollutants cause adverse health effects in humans and ecosystems. Due to rapid industrialization and urbanization, many pollutants have entered the environment, including pharmaceutical compounds, illicit drugs, pesticides, and personal



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care products. In addition, various per/polyfluoroalkyl substances (PFAS) have been found in many sources such as water, air, fish, soil, food, and food packaging, etc. Interestingly, PFAS degrade very slowly in the environment, which makes them one of the most important research topics for non-target environmental analysis. Liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS) have been used to analyze many pollutants in the environment. Many investigators reported that structural determination of ions can be achieved by high-resolution-MS, ion mobility spectrometry (IMS), and artificial intelligence. For example, one of the artificial intelligence tools is FluoroMatch, which is helpful for automated non-target analysis of PFAS. This workshop will discuss advances and challenges in the analysis of contaminants in the environment by non-target analysis, presented by several scientists in short overviews. This will be followed by a panel discussion led by researchers with relevant experience, along with active engagement of the audience. The goal is to share current experiences and knowledge about different instrumentation platforms for nontarget analysis of pollutants in the environment to stimulate further thinking and perspectives among researchers, as well as new artificial intelligence software packages, development of libraries of contaminants, sample preparation, and the benefits of 4D workflows, such as LC-IM-MS/MS.

14 Trans-Proteomic Pipeline: Recent Advances and Future Directions Independent Presiding: David Shteynberg, Michael Hoopmann Room 351CF

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on four 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 their challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topics for discussion will be focused on the new functionalities in the upcoming TPP version 6.3.0 release, including:

- Overview of the Cloud enabled TPP
- Cleavable crosslinker data analysis with Ving
- Integrating open searching into your usual workflow
- Mining for rare PTMs in your 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.

15 Imaging MS: Isomer Differentiation in Biological Imaging Imaging MS Interest Group Presiding: Ingela Lanekoff, Boone Prentice

Room 360ABDE

The differentiation of chemical isomers in mass spectrometry imaging can provide important information on biological processes. However, there are a number of limitations and challenges associated with separating and identifying isomers in conventional biological imaging workflows. A growing number of creative approaches and impressive methods have been reported recently, revealing new levels of chemical detail that provide novel insights into cellular biochemistry. Yet, the almost infinite number of isomeric compounds in biological systems suggests that additional efforts and tools are still required by the community. This workshop aims to discuss the current state of the field and the importance of defining the analyte with isomeric structural resolution. We also seek to highlight promising methods and paths forward that will increase the number of isomers that can separated in mass spectrometry imaging.

This workshop will be presented in two parts. First, several speakers will briefly describe their methodologies, including the pros and cons, for isomer differentiation in biological imaging. Second, the speakers will serve as a panel for a general discussion with the audience on the challenges that exist within the field, and identify opportunities and strategies for the future. The audience is encouraged to come prepared with questions and ideas.

16 Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing Independent Presiding: Gyorgy Vas, Kate Comstock

Room 360CF

Aspects of mass spectrometry support for extractables and leachables for pharmaceuticals and biocompatibility testing for medical devices will be discussed. Discussion will be focused on component identification and the required data support for component identification in the regulated environment. Another discussion topic would be non-targeted testing for biocompatibility, and leachables assessment.

17 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence Forensics & Homeland Security Interest Group Presiding: Ruth Smith, J. Tyler Davidson Room 361ABDE

Mass spectrometry is routinely used in forensic science for the characterization and identification of multiple different evidence types, ranging from seized drugs, to explosives, ignitable liquids, trace evidence, and even biological samples. Although GC-MS is perhaps the most widely used analytical technique, an increasing number of laboratories are implementing LC-MS/MS and DART-MS systems to enhance workflow and improve sensitivity. Given the continued complexity of forensic evidence submissions, even with these newer techniques, innovative approaches to mass spectral data analysis and data interpretation are needed.

This workshop will include a discussion of current challenges in forensic evidence analysis along with an overview of mass spectral tools developed by the National Institute of Standards and Technology (NIST). The panel will include forensic science practitioners who will discuss challenges within their area of expertise. Representatives from NIST will present various software tools that are freely available (e.g., AMDIS, MS Interpreter) and discuss ways that these tools can be employed to address the identified challenges. After the formal presentations, the moderators will facilitate an open-forum discussion in which workshop participants are encouraged to bring their own challenges for discussion.





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01 High throughput screening mass spectrometry - current status and future landscape Pharmaceuticals Interest Group

Presiding: Kiran Iyer, Jeremy Manheim

Room 310A

High throughput screening (HTS) systems provide the opportunity to measure several hundred thousand samples a day and is therefore in high demand in the pharmaceutical industry. Coupled to a sensitive and specific technique such as mass spectrometry (MS), HTS-MS systems are employed in several stages of the drug discovery process for applications that include, but not limited to, biomarker discovery, disease monitoring, targeted metabolomics, and the development of new chemical entities.

While there are several established MS platforms available for HTS, there are often constraints in trying to balance the throughput and the need for specialized equipment and custom-built software for data analysis. Some common HTS-MS platforms include the RapidFire-MS, multiplexed LC-MS/MS systems, Acoustic systems coupled to MS, MALDI-MS, and the more recently emerging HTS-DESI-MS systems.

This workshop aims to present:

- 1. The status on the use of HTS-MS systems for pharmaceutical analysis
- 2. Current developments, instrumentation, limitations and constraints with HTS-MS systems
- 3. Future outlook

The workshops aims to gather several presenters from instrumentation and pharmaceutical companies. Order of the presentations will be: 1) opening remarks from the presiders covering Topic 1, 2) two presentations from instrument companies (Bruker, Sciex) 3) two presentations from scientists in the pharmaceutical industry, and 4) closing remarks by the presiders. The audience for the workshop will be the industry community, researchers in academia, and analytical contract laboratories. Appropriate time will be designated to encourage participation and idea exchange with the audience. An expected outcome is to trigger the interest in the industry to embrace HTS-MS and for instrument companies to showcase exciting developments within this space.

02 Late-Night Lightning Lectures! Independent Presiding: Emily Sekera Room 310BC

This workshop will provide poster presenters a chance to present a 90-second lightning talk consisting of one slide maximum. This activity is intended to help challenge presenters to put their knowledge-translation skills to the test and gain experience presenting at a podium. It is our hope that the lightning talk will help speakers to garner interest in their posters during the week. Speakers will be chosen before the conference that cover a wide range of topics within ASMS. After the announcement of oral and poster presenters and confirmation of the workshop, we will send out a survey to aid in finding scientists interested in presenting. Preference will be given to speakers in labs who do not have an oral presentation at ASMS Houston 2023. Time permitting and level of interest, we will either conclude with a 15-minute open forum to allow audience members to give feedback to presenters and ask questions.

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03 Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory Flavors, Fragrance, and Foodstuff (FFF) Interest Group Presiding: Joe Binkley, Liz Humston-Fulmer

Room 320A

There are many challenging questions that a flavor, fragrance or food laboratory may be tasked to answer. These applications can include developing new products, deformulating competitive products, creating effective quality control methodologies, or identifying off odors and flavors, among many others. Addressing these challenges generally requires both hardware and software solutions. Due to the nature of many of the molecules responsible for a product's flavor and fragrance profile, GC/MS is frequently the hardware tool of choice. Once samples are analyzed, gleaning useful information from the rich GC-MS data is the next analytical challenge. Software tools that automate data processing and compile analyte information from the various samples can facilitate data review and improve efficiency for analytical scientists in this application field.

The goal of this workshop is to enhance attendees' knowledge about software tools which are available to make their day-to-day tasks easier and more efficient. Some of the software attributes which will be demonstrated during this workshop will include automated peak finding/identification, comparison strategies, and strategies for processing and comparing groups of samples. These demonstrations will serve as a starting point for a group discussion intended to engage and benefit attendees.

The workshop format will consist of two parts: 1) Panelists will provide brief examples and demonstrations of software tools which were used to effectively extract information from analytical data to solve real world problems in their laboratories. 2) Interactive discussion among attendees and panelists moderated by the interest group coordinators, including engagement with attendees by interactive, smartphone-based polling.

04 Biomarkers Development: How Mass Spectrometry Is Changing the Field Regulated Bioanalysis Interest Group Presiding: Wenkui Li, Jian Wang Room 320BC

A biomarker or biological marker is considered a measurable indicator of a certain biological state or disease related condition. Biomarkers are often evaluated qualitatively or quantitatively using blood, urine or tissues to examine normal biological processes, pathogenic processes, or pharmacologic responses to a therapeutic intervention. LC-MS is a powerful analytical tool for the analysis of various biomarkers including small molecule and large molecule biomarkers. This workshop is to be featured by presentations covering LC-MS biomarker analysis- 'When? How? Why? hybrid LC-MS for protein biomarker quantitation, use of a universal surrogate matrix assay for biomarker analysis, and quantitative target occupancy analysis using immunoaffinity capture 2D-LC-MS/MS, etc.

This workshop will develop future discussions and consensus on LC-MS biomarker analysis in support of regulated studies, including topics on sample preparation, mass spectrometric methods and data processing. Experts in the field will share their experience in this highly interactive workshop.



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05 Ion Mobility Spectrometry: From Data to Structure Ion Mobility MS Interest Group Presiding: James Prell, Xueyun Zheng

Ballroom A

In addition to separating isobaric analyte ions and increasing peak capacity, Ion Mobility (IM) Spectrometry can often help characterize ion structure. However, the drift time/collision cross section (CCS)-ion structure relationship can be complicated, whether in predicting a CCS from a model structure or vice versa. State-ofthe-art methods for these tasks range from using detailed physical modeling of the ion-gas scattering process to using Machine Learning based on molecular descriptors and experimental CCS databases. These methods differ in their emphasis on the parent condensed-phase structure versus structure after transfer into the gas-phase environment. This workshop aims to stimulate discussion about the advantages and challenges of a range of strategies for structural interpretation of IM-MS data. After a brief (5 minute) introduction to the problem of relating IM-MS data to ion structure by the presiders, we will feature perspectives spanning industry and academic research, as well as empirical versus first-principles approaches. We aim to invite a panel of speakers that are working on different approaches, such as conventional "frozen-structure" scattering models. Machine Learning/ molecular descriptor-based approaches, and molecular dynamics approaches. Example topics of discussion include: When might it be useful to understand the structures of gas-phase ions, if they have changed significantly from those in the condensed phase? Should we focus in the future on more accurate scattering models or on improving predictive capabilities of molecular descriptors? How can these approaches learn from each other?

06 MS Career Options: How to Kick Start Your Career Young Mass Spectrometrists Interest Group Presiding: Christopher Pulliam, Ryan Bain Ballroom B

Description: The Young Mass Spectrometrists workshop focuses on a panel discussion where representatives of various careers paths discuss their journey to their current position and answer questions regarding their current and past experiences. Through this discussion mass spectrometrists at the undergrad, graduate, or postdoctoral stage of their career learn information or strategies that will help them navigate the next steps in their career. This panel typically comprises representatives from a wide swath including academia, biotech/pharma, start-up companies, government, and non-traditional career paths to provide a comprehensive view of career opportunities for young researchers who have mass spectrometry skills.

07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided? Ambient Sampling & Ionization Interest Group Presiding: Chris Gill, Roshan Javanshad, Jacob Jordan Ballroom C

Ambient ionization mass spectrometry has been a durable topic at ASMS since 2006 ("Direct Ionization Techniques"). Since the first workshop in 2019, it has been a great platform for attendees to discuss innovations and issues in instrumentation, sampling, ionization, and related applications, as well as the underlying scientific mechanisms. In recent years (2021, 22), this workshop had 50 and 86 attendees from academia, industry, and government. At the first workshop in 2019, concerns and interest in the field were polled from some 200 attendees. The workshops in the following years have responded to the interests of our community, with foci of "reproducibility, 2020", "quantitation, 2021", and "molecular coverage, 2022".

This year, the workshop will highlight the applications of ambient ionization while continuing our discussion of these figure of merit (FoM) topics. The versatility of ambient ionization methods makes mass spectrometry approaches more accessible in a wide range of areas including forensics, security, environmental analysis, manufacturing, imaging, and clinical/point-of-care diagnostics. Each application has a set of different desired and required FoMs for analytical methods. Besides exhibiting the state of the art in these areas via lightning talks, the workshop will survey these FoMs in relevant applications. Attendees will put stickers on a prepared poster (like in 2019) to indicate the desired FoMs (sensitivity, accuracy, molecular, etc.) in their application/areas. Expert panelists will lead a Q&A-style discussion that covers challenging aspects, recent breakthroughs, and potential research directions in our research community.

08 Target Protein Degradation and MS-based Proteomics Independent Presiding: Pankaj Dwivedi Room 3332

Target Protein Degradation (TPD) research field is evolving rapidly. Given proteins are the functional unit of the cell, it is very promising to target "bad" proteins in the cell with respect to finding a potential therapeutic avenue for certain disease. Proteomics has always been instrumental in understanding of the normal and disease biology. This workshop is dedicated to understanding/ active discussion regarding the opportunities and challenges associated to MS-based proteomics for TPD.

09 What are the future needs of photoionization mass spectrometry for complex mixture analysis? *Photoionization MS* Presiding: Christopher Rüger General Assembly A

Photoionization schemes for mass spectrometry, either by laser or discharge lamps, have been widely examined and deployed for almost every application area and field of science. Fundamentals on the reaction mechanisms for atmospheric pressure photoionization (APPI) have been described in the early 2000s. Different manufacturers developed and launched APPI sources commercially, and various research groups published on specific geometries and designs. However, APPI development has been largely halted, and APLI has fallen into a niche without major commercialization. Consequently, this workshop aims to address the future needs for APPI development and potential application areas in complex mixture characterization from the fields of environmental and material sciences as well as energy transition. Questions are raised for: What are the light sources utilized in the mass spectrometry market for photoionization? What novel light sources are available and might be handy in mass spectrometry, such as innovative laser concepts, e.g., OPO? What are photoionization's unique chemical application fields and benefits, and how can this be combined with established ESI/APCI workflows.? The workshop will feature different short presentations to initiate a discussion atmosphere.



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10 Houston, We Have a Microbiome Problem (...and how the Metaproteomics Initiative aims to solve it!)

Independent

Presiding: Pratik Jagtap, Robert Hettich, Timothy Griffin, Tim Van Den Bossche

General Assembly B

Mass spectrometry-based metaproteomics research has experienced rapid growth due to its ability to help characterize complex microbial communities and is likely to become a central approach for understanding how microbiomes function. Despite its value, metaproteomics offers analytical and bioinformatic challenges beyond those encountered in traditional, singleorganism MS-base proteomics. As a solution, the Metaproteomics Initiative (www.metaproteomics.org) is a global initiative that promotes the dissemination of metaproteomics fundamentals, analytical and bioinformatic advancements, and microbiome applications. Members of the Initiative will present the updates on two recent CAMPI (Critical Assessment of Metaproteome Investigation) benchmark studies on sample preparation and functional annotations, and future projects that will be designed to propel this field forward. The members will also provide highlights from the 5th International Metaproteomics Symposium (Avignon, France), which was held in April 2023.

The workshop will invite a panel of leading metaproteomics experts who will participate in a discussion that covers the status of metaproteomics, research needs, and growth opportunities. The panel will also interact with the audience and address discussion points on how the initiative will help in gaining deeper insights into microbiome dynamics. The workshop will also describe the Initiative along with information on how interested researchers can join, participate, and contribute to its growth.

11 Hispanics and Latinx in Mass Spectrometry Independent

Presiding: Benjamin Garcia, Livia Eberlin, Francisco Fernandez Lima

General Assembly C

This workshop proposal looks to organize the first official meeting of the newly forming Hispanics and Latinx in Mass Spectrometry outside interest group. Since 2003, Hispanics/Latinx have been one of the largest growing minority groups in the United States population. Nevertheless, this has not been reflected in our ASMS community membership of scientists. According to the ASMS demographic data, Hispanics/Latinx only comprise ~3% of the scientist membership, well under the U.S. population average. In order to continue to support and grow this important group, several Hispanic/Latinx scientists have come together to begin to form a new outside interest group. It is our hope that by becoming more visible and active at ASMS Conferences and beyond, we can encourage the younger Hispanic/Latinx scientists to become more involved in the mass spectrometry field. Specifically for this workshop at the ASMS Conference, we plan to have an event where we will showcase the research that Hispanic/Latinx scientists are currently engaging in, making sure to highlight the younger members of our society. It is hoped that in addition to the cutting-edge research, the speakers will also discuss their personal journeys that got them to this point in their careers. Additionally, we'd like to spend some time to have an open panel discussion to give the opportunity to our audience to ask questions, and also to solicit ideas and feedback on how

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this new outside interest group can be more effective to organize, outreach and grow. It is anticipated that this workshop will be the first event catalyst to encourage and support the Hispanic/ Latinx members of ASMS. This workshop is open to anyone who identifies as Hispanic/Latinx in any way, and also to members who have trainees/co-workers from these groups as well (Allies).

12 Polymeric materials: tackling hydrocarbon-based polymers

Polymeric Materials Interest Group Presiding: Thierry Fouquet, Anthony Gies Room 340AB

Following a brief introduction on the interest group business (application for Sanibel/Asilomar conference, informal meetings), we will start out discussing the analysis of hydrocarbon polymers with one presentation from a member (10-15 min). The presentation will include a brief overview of existing MS techniques for the microstructure analysis of styrenic and olefinic polymers and cover the current limitations / possible solutions to explore. Attendees are invited to ask questions throughout the presentation. The main part of the workshop will then take the form of a live session of data processing using commercial and free programs for the exploration of complex MS and MS/MS data. The hosts (one or both organizers, at least one more invited presenter) will provide examples to show the advantages of advanced data analysis approaches. Attendees are encouraged to share their own datafiles in advance - or during the workshop to spice up the demonstration - to help drive the interactivity. Such a live demonstration (at least 40 min) will be the first of its kind for our interest group and will undoubtedly trigger fruitful discussions among members. It is envisioned that the flow of ideas will enable the development of new data analysis tools or pinpoint the need to modify preexisting software solutions. The final discussion (typically 15 minutes) will be focused on the potential use of ion mobility to complement MS for the detailed characterization of these highly complex polymeric materials (tentative topic), and/or any topic attendees may wish to tackle, e.g. via the presentation of a single slide of their results/ideas.

13 ProteomicsML: An online educational platform for machine learning in proteomics Independent Presiding: Juan Antonio Vizcaíno

Room 351ABDE

Open data science practices in proteomics have been largely driven by the efforts of the Proteomics Standards Initiative (PSI, http://www.psidev.info) and the ProteomeXchange Consortium of proteomics resources (http://www.proteomexchange.org). Both are two highly collaborative community initiatives that are open to the contribution and ideas from everyone. Since 2002, the mission of the PSI is the development and promotion of open data standards and related software in the proteomics field. Some recent and ongoing projects are focused on the development of a standard format for spectral libraries (mzSpecLib), the standard notation ProForma 2.0 for peptidoforms and proteoforms and the Universal Spectrum Identifiers, apart from updates in other widely adopted formats such as mzML and mzIdentML. In a parallel effort, since 2012, the ProteomeXchange Consortium is standardising the submission and dissemination of public proteomics data between the main proteomics data repositories,



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currently including the resources PRIDE, PeptideAtlas, MassIVE, jPOST, iProx and Panorama Public.

We will briefly highlight current trends in the increasing re-use of public proteomics datasets. As a key recent output of open science practices in the field, we will highlight the ProteomicsML platform (https://proteomicsml.org/). ProteomicsML provides ready-made datasets for machine learning models accompanied by tutorials on how to work with even the most complex data types. The resource is set up to evolve together with the field, and we welcome everyone to contribute to the project by adding new datasets and accompanying notebooks.

14 Art, Museums, and Archaeology Independent Presiding: G. Asher Newsome, Paul A. Haynes Room 351CF

The study of artworks, archaeological specimens, and other cultural heritage objects by mass spectrometry requires the adaptation of previously developed techniques, as well as the development of new approaches. Analytical methods used in biomedicine, industrial and natural product research, and forensics must be carefully tailored to be successfully applied in diverse fields such as anthropology, archaeology, natural history, art history, paleontology, and more. This multidisciplinary workshop will feature lightning talks selected from ASMS poster abstracts - students and fellows are encouraged to volunteer in advance by contacting the organizers. Lightning talks will be followed by audience Q&A with a panel of academic, government, and private institution scientists to discuss areas of interest in the field. This will provide a great opportunity to exchange detailed information about essential methodology which is often excluded from published literature. Science and science-adjacent topics may include: ethics and permissions involved in analyzing culturally sensitive samples; the risk of damage to objects as a result of analysis; sample-limited preparation and recovery approaches for rare and precious analytes; considerations for historical and contemporary sample contamination; the significance of preservation and prediction of material degradation; discerning the importance of chemicals identified from an analyte removed from context; employment, funding, and fellowship opportunities; and many more.

15 Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions Independent

Presiding: Donald Chace, Timothy Garrett Room 360ABDE

Large volumes of blood, urine and other biological fluids (1mL or more) are becoming more obsolete and impractical in clinical chemistry practice with the exception of the inpatient environment (hospital). There is a shift in demand for sampling outside of the hospital or clinic because of concerns regarding access, rise in telemedicine, and the desire for direct to patient solutions. The covid pandemic likely accelerated this sea change in biological fluid sampling. Remote sampling of biological fluids relies on volumes that are much smaller roughly defined as less than 1 ml and typically is in the range of 50- 300 uL needed on average during collection. This microsample can be either liquid (wet) or a dried in a matrix such as paper. Newborn screening has used the dried microsample for more than 50 years as part of its sample collection format from newborns. The analysis of these DBS includes many classical clinical chemistry methods as well as mass spectrometry (specifically tandem MS).

The are many issues facing microsampling in terms of precision and accuracy of such small volumes whether they are wet or dry. For mass spec, an inherently selective and accurate measurement device, precision is important as well as detection limits, limits of quantification etc. Further automation of sampling handling, interpretation are all issues that are important, many of which were identified in newborn screening. Microsampling has numerous advantages but also challenges that are being addressed.

This interest group will be focused on best practice for microsampling from isotope dilution MS, standardization, recovery from the matrix, analyte stability, suitability for analysis. It is a rapidly evolving field for which mass spec is a key player from small molecule to proteins. Cost and convenience is a huge driver of this technology as well and this group should attract a good attendance.

16 Knowledge Share and Instrumentation Donations for Developing World Outreach Developing World Outreach Interest Group Presiding: Giles Edwards, Kym Faull

Room 360CF

This new ASMS Special Interest Group (SIG) aspires to bring together those who wish to share their ideas on how we as a society can assist in deploying mass spectrometry as a key analytical technique to address educational, health, environmental and economic issues in the Developing World. The idea to establish this SIG stemmed from workshops entitled "Mass Spectrometry in the Developing World: supporting education and research", held for the past three years at the annual ASMS meetings. Future correspondence will address the items on the agenda to be addressed. For now, we invite all interested ASMS members to join the SIG and follow the postings on this site.

The organizing committee of this group have shipped and installed a number of mass spectrometry products in developing countries for academia. If any ASMS members would like to contribute redundant instrumentation, their engineering or applications based knowledge it would be gratefully received. The group aims to work out a strategy to utilize the skill set of ASMS members for outreach activities.





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