73rd ASMS Conference on Mass Spectrometry & Allied Topics, June 1 – 5, 2025
MONDAY NETWORKING SESSION & EVENING WORKSHOPS

MONDAY NETWORKING SESSION, 12:00 - 1:00 pm

Networking Session: Celebrating Women Mass Spectrometrists

Presiders: Tian (Autumn) Qiu, Prasanna Ashok Kumaar, Rosangela Silva Santos

Poster-Exhibit Hall, 12:00-1:00 pm

Come celebrate and be empowered by the journey and success of women mass spectrometrists in this networking event, organized in collaboration with Females in Mass Spectrometry!

- The session opens with a keynote presentation by a notable guest speaker, sharing career insights and stories of encouragement.
- The session continues with interactive discussions with the keynote speaker and invited guests from various career stages. Participants will have the opportunity to ask questions and to pose comments via an online platform or feel free to raise your hand!
- Of course, the session will feature networking time in small groups with trailblazers from the mass spectrometry community.

We invite all to join us in this 8th edition of the networking session on Celebrating Women Mass Spectrometrists – build meaningful connections and find inspirations to navigate your career.

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

01 Career Paths for Mass Spectrometrists: A Speed Networking Workshop

Career Development Interest Group

Presiders: Olya Vvedenskaya, Rosangela Silva Santos

Room 307-308

Career development in mass spectrometry offers diverse opportunities across academia, industry, government, and communication. However, navigating these paths and making informed career choices can be challenging for early career researchers.

This interactive workshop, organized in collaboration with the FeMS+ community, provides an opportunity to engage directly with professionals representing the following career trajectories:

- Government research - A senior research scientist working in a governmental agency – Dr. Maggie Tam
- Core facility management - A director of a mass spectrometry core facility – Dr. Prasanna Ashok Kumaar
- Science communication - A science communicator working in a biotech company – Dr. Olya Vvedenskaya
- Industry applications - A leader of an omics direction at a vendor company – Dr. Erica Forsberg
- Academic research - A postdoctoral researcher at a university – Dr. Duong Bui

The 90-minute session will begin with a brief introduction to the format, followed by five-minute presentations from each expert on their career journey and day-to-day responsibilities. Attendees will then participate in two 25-minute roundtable Q&A sessions, where they can rotate between speakers to ask questions. The event will conclude with a summary of key takeaways and networking opportunities.

This workshop is ideal for students, postdocs, and early-career scientists looking to explore different career options in mass spectrometry.

02 Real time Mass Spectrometry in Proteomics and Beyond

Independent

Presiders: Devin Schweppe**,** Nick Riley**,** William Barshop

Room 309-310

'Real-time mass spectrometry is the analysis or interpretation of spectral data in parallel with instrument acquisition to inform, optimize, or control future spectral acquisition.' The democratization of real-time instrument control is enabled by recent instrument application programming interfaces and has led directly to new methods for targeted (MaxQuant.Live, PRMlive, GoDig) and discovery proteomics (real-time search, real-time library search).

The purpose of this workshop is to provide a foundational demonstration of state-of-the-art real-time instrument control through short presentations (5-15 minutes) by invited experts. These presentations lay the groundwork for a panel discussion (30 minutes) that segues into an informal discussion on emerging topics for real-time instrument control (30 minutes). The format offers a unique and exciting opportunity to engage in open discussion, support junior researchers, and identify gaps in the current field that lab- or community-lead efforts can address. The workshop will establish avenues to improve open sharing of data, code, documentation, and methods for the continued development new real-time mass spectrometry tools.

03 Chemoproteomics: The Next Frontier for Drug Development (and More)

Independent

Presiders: Keriann Backus**,** Lindsay Pino

Room 314-317

Chemoproteomics has emerged as a critical discipline at the intersection of chemistry, proteomics, and drug development. As advances in chemical biology and mass spectrometry continue to accelerate, the opportunities for elucidating complex biological processes and identifying potential therapeutic targets have expanded tremendously. Building upon our 2024 workshop, we seek to bring together leaders and researchers in chemoproteomics from academia and industry to exchange knowledge, perspectives, and experiences. The workshop will focus on recent breakthroughs, methodologies, and technological innovations driving advancements in chemoproteomics and its application in the biomedical and drug discovery fields. The workshop will begin with a short introduction, “what is chemproteomics,” by the presiders followed by a panel discussion with a mix of industry and academia experts giving their "hot takes" and debates on the topic. Panelists will focus on the state-of-the-art for chemoproteomics as well as ongoing challenges and opportunities, spanning chemical tools, sample preparation, and data acquisition and analysis. By exploring and discussing the latest developments in this dynamic field this workshop aims to foster collaboration, share insights, and spur future innovation.

04 Benchmarking Datasets for Untargeted Metabolomics and Exposomics and Compound Identification

Metabolomics Interest Group

Presiders: Corey Broeckling, Xiuxia Du

Ballroom II

Evaluation of software tools for untargeted mass spectrometry (MS)-based metabolomics and exposomics requires benchmarking datasets to ensure rigor and objectivity. This workshop will feature two datasets that have been created to address this need. The first dataset is for evaluating software tools that extract compound information from raw MS data. The second dataset is for the discovery and identification of molecules.

To produce the first benchmarking dataset, samples were prepared that consist of three pairs of reagents: (1) Standard mixtures of 96 pure analytes (96Mix); (2) Commercially available yeast cell extract containing separate 12C and uniformly 13C-labeled samples that were prepared in parallel; and (3) human plasma SRM 1950 paired with SRM 8231. These complex reagents have been mixed in a systematic and highly structured manner to enable objective heuristic rules to serve as ground-truths. All of the data were acquired on a Waters Acquity coupled to a Q-TOF and a UHPLC coupled with Orbitrap ID-X. Samples were separated using both HILIC and reverse phase chromatography, and profile data acquired in both positive and negative ionization mode. Data were acquired in MS only mode, and additional injections were performed in DDA MS/MS mode. The second benchmark dataset comprises the largest publicly available collection of high-quality labeled MS/MS spectra.

At this workshop, we will introduce these two datasets and conduct a survey to seek feedback from the audience to better understand the needs of the metabolomics and exposomics community to make metabolomics and exposomics informatics tools more rigorous and transparent.

05 Top-Down Proteomics: Software and Data Analysis Strategies for Getting the Most Out of Your Data

Top-Down Proteomics Interest Group

Presiders: Corinne Lutomski, Fanny Caroline Liu

Ballroom I

Despite ongoing advances in technology, the field of top-down proteomics (TDP) still faces significant challenges obstructing widespread adaptation. These obstacles span across all stages of the experimental workflow, including sample preparation, protein ionization/fragmentation, and data analysis. While efforts to democratize sample preparation and fragmentation have recently been published through community studies, data analysis remains a significant bottleneck in the widespread adaptation of TDP. A survey among the audience at the 2023 top-down proteomics workshop at ASMS indicated a critical challenge remains in software and data analysis.

This workshop will provide insight toward applying TDP to targeted analysis in biomedical, biopharmaceutical, and academic applications with a special focus on fully interpreting the complex data generated in TDMS experiments. The goal of the workshop is to provide perspectives from a range of experts in native and denatured top-down MS to provide a foundation for interpreting top-down spectra. The workshop will host six panelists, each panelist will give a short introduction about how they use top-down proteomics, the strategies they use to interpret top-down data, and the key metrics they look for. The audience will be directed toward resources for data analysis, including both free and commercial software packages.

06 Latest Developments in Open Data Standards Practices in Proteomics

Independent

Presiders: Douwe Schulte, Wout Bittremieux, Petr Novák

Ballroom III

The Proteomics Standards Initiative (PSI) has openly and collaboratively developed mass spectrometry data standards since 2002. This workshop will introduce some recent standards, ProForma 2.1, mzPAF, mzSpecLib, and Universal Spectrum Identifier (USI), and show their applicability to annotate MS2 spectra. The session will be closed with a discussion on the applicability and issues of the standards for the wider community.

The workshop will start with a plenary introduction of the ProForma notation. A notation to write down definitions of complex peptidoforms, explicitly supporting bottom-up, top-down and many other fields of mass spectrometry. We will address its recent update but focus on how to use it in common cases. This introduction will be alternated with hands on applying the introduced concepts in Annotator, a highly customisable fragmentation annotator for any proteomics MS data. By having these hands-on sections we can teach how to use ProForma in practice.

After the introduction of ProForma we will introduce Universal Spectrum Identifiers, which can be used to easily visualise publicly available mass spectra in the ProteomeXchange data ecosystem, e.g. the PRIDE database. This again will be alternating between plenary instruction and hands-on sections with the same software.

The session will end with a short recap of what was introduced and a discussion on the bottlenecks for applying the shown formats more generally. This section's goal is to find use cases for these formats not currently enacted and fields for which these formats do not have the necessary expressiveness to be of use.

07 Towards Guidelines for DIA Reporting Criteria

Data Independent Acquisition Interest Group

Presiders: Mike MacCoss, Michael Ford

Ballroom IV

The guidelines for reporting mass spectrometry proteomics data were outlined over twenty years ago and have provided a solid calibrator for the field since that time[1]. DIA specific guidelines were suggested in 2019[2]. It is our thought that an update to these guidelines may be necessary to include properties unique to evolving DIA workflows. The purpose of this workshop is to provide a forum for the discussion of DIA reporting guidelines. In an informal but structured setting of an ASMS workshop the community can engage in an open discussion about how the criteria may look and be applied. It is our intention to engage several experts in the field before the meeting to 1) establish a highly qualified list of speakers and 2) outline a set of goals/discussion points to ensure a focused conversation.

We hope for a lively discussion with community engagement. A framework for updating the reporting guidelines may emerge.

- The Need for Guidelines in Publication of Peptide and Protein Identification Data. Carr, Steven et al. Molecular & Cellular Proteomics, Volume 3, Issue 6, 531 - 533

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

- Initial Guidelines for Manuscripts Employing Data-independent Acquisition Mass Spectrometry for Proteomic Analysis. Chalkley, Robert et al. Molecular & Cellular Proteomics, Volume 18, Issue 1, P1-2

08 MS Outreach: Knowledge Share and Instrumentation Donations

Developing World Outreach Interest Group
Presiders: Hendrik Kersten, Giles Edwards
Room 336

The ASMS Interest Group "Developing World Outreach" 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 organizing committee of this group has shipped and installed a number of mass spectrometry products across the Globe for academia. If any ASMS members would like to contribute 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.

Recently, this group has setup a MS Online Seminar to facilitate academics, engineers and enthusiasts to share their research and mass spectrometry experience with others across the Globe (https://www.ipams.uni-wuppertal.de/de/startseite/workshops/conferences/online-ms-seminars).

The seminar sessions are free of charge and we would like to encourage ASMS members to join, present and get in touch with scientists around the globe who do not necessarily have the financial means to attend a conference like this one. Sharing is caring.

09 Taste to Targets: Food, Flavor and Fragrance Workshop

Flavor Fragrance & Foodstuff Interest Group
Presiders: David Schroeder, Devin Peterson, Candice Ulmer Holland
Room 339-340

Food Flavor and Fagerance tools, techniques, and strategies discussion focused on applications.

Work Group discussion primers:

- Beer and coffee flavor analysis case studies for by Flavor Research and Education Consortium.
- USDA nutritional, residue chemistry, and Siluriformes
- Panel expertise SAFE, Dynamic Headspace, GC x GC, GC-MS/MS, GC-ToF LC-MS, LC-ToF

10 Nitrosamine Analysis in Pharmaceutics: Evolving Challenges and Emerging Solutions

Pharmaceuticals Interest Group
Presiders: Paolo Lecchi, Mack Shih, Jessica Hoskins
Room 341-342

Following the success of last year's workshop on nitrosamines, this session will provide an update on recent developments in the detection and quantification of nitrosamine impurities in pharmaceutical preparations. With evolving regulatory expectations and scientific advancements, the need for reliable analytical strategies remains critical.

This highly interactive workshop will foster open discussions and knowledge sharing among participants. Experts from various sectors will present the latest advancements in analytical methodologies, regulatory considerations, and industry best practices. Attendees will have the opportunity to engage in dynamic discussions, share experiences, and explore practical solutions to common challenges in nitrosamine analysis.

Through case studies, Q&A sessions, and group discussions, participants will engage in an open and interactive exchange on method development, validation, and risk assessment strategies. This session will provide a collaborative forum for discussing challenges, sharing experiences, and exploring current approaches to nitrosamine detection and quantification in pharmaceutical preparations.

11 Mass Spectrometry in Quality Control for Complex Biotherapeutics Modalities

Biotherapeutics Interest Group
Presiders: Sara Carillo, Sarah Rogstad
Room 343-344

The biotherapeutic landscape is seeing the rapid emergence of therapeutic formats more complex than traditional monoclonal antibodies as entities such as antibody drug conjugates (ADCs), bispecific antibodies (bsAbs), and fusion proteins. While these formats offer distinctive advantages in targeting diseases and are among the most promising drug classes in oncology, they pose new challenges from both design and quality control points of view.

Mass spectrometry techniques provide an attractive tool to decipher some of the critical quality attributes (CQAs) of these complex modalities and as such can be implemented in a Quality by Design (QbD) aspect of their development towards commercialization. However, minimal instances of mass spectrometry in QC have been approved for therapeutic proteins, and even fewer for complex modalities. When mass spectrometry has been implemented for these products, the specific approaches and CQAs analyzed have varied widely.

This workshop aims to: 1) understand current best practices in CQA analysis and monitoring for complex biotherapeutic modalities, 2) highlight the benefits of mass spectrometry-based analysis for ADCs, bsAbs, and fusion proteins, and 3) understand the technical and practical limits for their implementation in QC.

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

12 Photoionization MS: Where It Excels, Where It Falls Short, and How It Complements Other Methods

Photoionization MS Interest Group
Presiders: Christopher Rüger, Sven Ehlert, Patrick Mueller
Room 345-346

Photoionization mass spectrometry (PI-MS) has emerged as a powerful analytical tool, offering soft ionization with minimal fragmentation, high selectivity, and real-time analytical capabilities. It is particularly well-suited for volatile and semi-volatile compounds, allowing for direct analysis without the need for extensive sample preparation. However, its role within the broader landscape of ionization techniques remains a topic of active discussion. How does PI-MS compare to and complement traditional ionization techniques such as electron ionization (EI), electrospray ionization (ESI), and atmospheric pressure chemical ionization (APCI)? What are its limitations in terms of ionization efficiency, matrix effects, and compound coverage, and where does it offer unique analytical advantages?

This engaging workshop, hosted by the Photoionization Mass Spectrometry Interest Group, will feature three 5-minute flash talks offering focused insights into different aspects of PI-MS and its interplay with other ionization techniques. Discussions will explore hybrid ionization approaches, where PI-MS is coupled with complementary sources to enhance molecular coverage, as well as its application in real-time environmental monitoring, metabolomics, and high-throughput analysis.

A podium discussion will bring together experts to debate key topics, including ion source flexibility, selectivity vs. sensitivity trade-offs, and the integration of PI-MS into multi-technique workflows. Panelists will also deliver bold "Hot Takes" on the future of PI-MS, its evolving applications, and its potential role in next-generation analytical instrumentation.

The session will conclude with an open discussion and audience Q&A, offering attendees a unique opportunity to exchange ideas, discuss practical challenges, and explore innovative strategies for implementing PI-MS in modern analytical workflows.

13 Undergraduate Research: Strategies for Success

Undergraduate Research in MS Interest Group
Presiders: Mac Gilliland, Micah Donor
Room 347-348

Undergraduate research experiences can be exceedingly valuable, to both the students and their mentors, yet there are many unique challenges associated with them. In this workshop we will explore practical strategies for creating successful and productive undergraduate research experiences. From lab startup to regular operation, from project idea to publication, we will discuss key aspects of undergraduate research. This will include: making the most of limited time; working during the summer vs. during the academic year; recruiting and training new researchers; mentoring students with diverse backgrounds; developing independence; maintaining continuity from student-to-student; and involving students in the publication process. We expect that this workshop will be particularly useful to undergraduate students and anyone who mentors undergraduates - including PIs, postdocs, graduate students, and career scientists. This workshop will be highly interactive, with space for attendees to contribute their perspectives on these topics and participate in a discussion of how this group can best foster a strong culture of undergraduate research within ASMS.

14 Environmental Applications: You Are What You Eat and Breathe

Environmental Applications Interest Group
Presiders: Erin Baker, Carrie McDonough
Room 349-350

Chemicals in the environment have a massive impact on our health and well-being. For the many chemicals we are exposed to daily through ingestion, inhalation and dermal absorption, their health impacts are unknown. However, from Paracelsus we know that "the dose makes the poison", and any chemical, even water, can be toxic if consumed at high enough amounts. In this workshop, the audience will test their knowledge on the history and current state of chemicals of concern through an interactive quiz (with prizes!!). We will then have several short talks on current developments in environmental measurement approaches and applications, such as novel non-targeted analysis developments and computational workflows, which are allowing us to probe new chemicals of concern that we did not even know existed.