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# 38<sup>th</sup> Asilomar Conference on Mass Spectrometry

## COMPUTATIONAL MASS SPECTROMETRY

Friday, October 13 - Tuesday, October 17, 2023  
Asilomar Conference Center, Pacific Grove, CA

### Organizers

**Nuno Bandeira**, *University of California, San Diego*

**David Fenyö**, *NYU Langone Medical Center*

**Olga Vitek**, *Northeastern University*

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### ASMS Asilomar Committee

**Chris Anderton**

*Pacific Northwest National Laboratory*

**John Bowden**

*University of Florida*

**Laura Sanchez**

*University of California, Santa Cruz*

**Susan Richardson**, ASMS Board Representative

*University of South Carolina*

## NOTES

## GENERAL INFORMATION

### INTERNET / WiFi ACCESS

There is complimentary wi-fi access in the session room (Chapel). This is different than the guest room network.

- Connect to network: **Asilomar Conference**
- Enter Promotional Code: **Asilomar2023**  
(capital A, no spaces)
- Accept the terms & conditions

### HANDS-ON TUTORIAL, FRI 3:30-5:30 PM Superior Routes to mzML for Bruker timsTOF and SCIEX TripleTOF in Fast Photochemical Oxidation of Proteins

Files for advance download (before you travel) are strongly recommended. Look for email from [info@asms.org](mailto:info@asms.org) for instructions to download the materials.

### MEALS AT ASILOMAR

For attendees lodging at Asilomar you will receive meal tickets for all meals beginning with dinner on Friday and ending with lunch on Tuesday. A vegetarian option is always available upon request at the meal line. *For Tuesday a box lunch has been requested for you, please use your remaining lunch ticket to pick up your box lunch on Tuesday morning, 7:45-9:00 am in Crocker Dining Hall.*

For attendees staying offsite you will have (3) lunch tickets. If for some reason you did **not** pay the offsite fee, there will be no tickets for you at registration. If you also purchased any dinner tickets they will also be available to you at registration.

All meals are available as "To-Go". You can take your "To-Go" meal to the beach or find a nice perch on the campus.

### EVENING RECEPTIONS

Friday, Saturday, and Sunday evenings an informal reception in Chapel immediately following the evening session. These evening mixers are an opportunity to continue lively discussion and interact with fellow attendees.

### SUNDAY AFTERNOON

There is a free afternoon. Attendees are encouraged to join others for outings. Suggest your own activity or sign up to join others. Sign-up sheets in Chapel (session room).

### MONDAY EVENING

Weather permitting, we will have a bonfire with s'mores at the firepit outside of Crocker Dining Hall following the final session on Monday. If you do not know what a s'more is, we will show you!

### PRESENTER GUIDELINES

Invited Speakers and Short Talk Speakers. Please arrive in the Chapel 15-20 minutes prior to the start of the session to set up your device or load your presentation onto the conference computer (PC). Remember to have your own adapters handy to connect to HDMI if using your own device.

Poster Presenters. Mount posters by 6 pm Fri (or as soon as you arrive). Remove after Monday evening closing session (or just before panel discussion).

Poster Highlight Talks. Follow instructions you received by email. Please send slides for your talk to [jennifer@asms.org](mailto:jennifer@asms.org) by 1:00 pm on Saturday, Oct. 14.

### PROGRAM OVERVIEW

#### Friday

3:00 - 6:00 pm.....Badge Pick-up  
3:30 - 5:30 pm.....Hands-On Tutorial  
6:00 - 7:00 pm.....Asilomar Dinner  
7:15 - 8:15 pm.....Opening Session  
8:15 - 9:30 pm.....Reception & Posters

#### Saturday

7:30 - 9:00 am.....Asilomar Breakfast  
9:00 am - 12:00 pm.....Session  
12:00 - 1:00 pm.....Asilomar Lunch  
1:15 - 3:10 pm.....Session  
3:10 - 3:15 pm.....Group Photo  
4:00 - 5:30 pm.....Session  
6:00 - 7:00 pm.....Asilomar Dinner  
7:15 - 7:50 pm.....Session  
7:50 - 9:30 pm.....Reception & Posters

#### Sunday

7:30 - 9:00 am.....Asilomar Breakfast  
9:00 am - 12 pm.....Session  
12:00 - 1:00 pm.....Asilomar Lunch  
1:00 - 6:00 pm.....Free Afternoon  
6:00 - 7:00 pm.....Asilomar Dinner  
7:15 - 8:00 pm.....Panel Discussion  
8:00 - 9:30 pm.....Reception & Posters

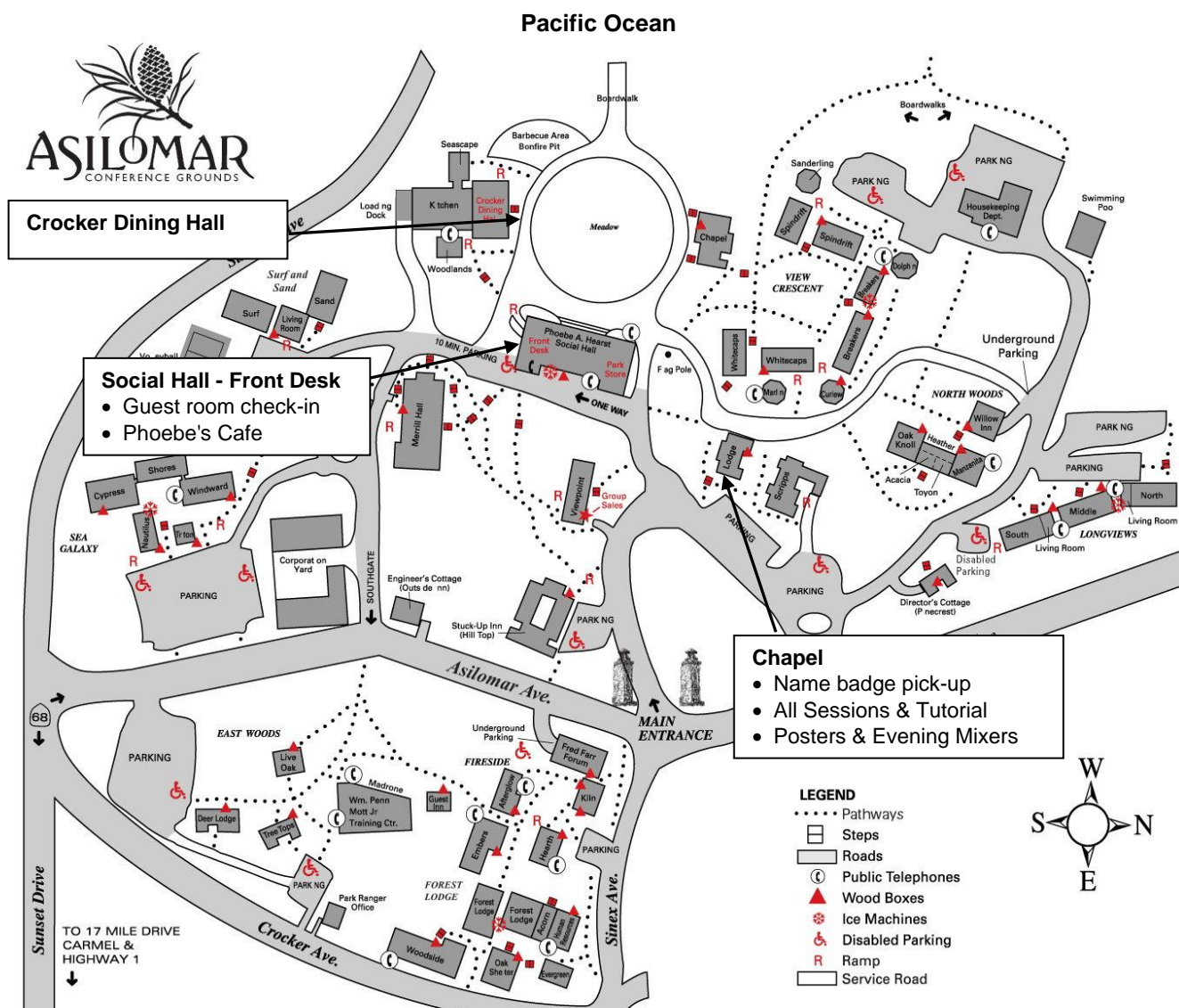
#### Monday

7:30 - 9:00 am.....Asilomar Breakfast  
9:00 - 11:50 am.....Sessions  
12:00 - 1:00 pm.....Asilomar Lunch  
1:15 - 4:00 pm.....Sessions  
4:00 - 6:00 pm.....Free Time  
6:00 - 7:00 pm.....Asilomar Dinner  
7:15 - 8:00 pm.....Panel Discussion  
8:25 - 10:00 pm.....Bonfire & S'Mores!

#### Tuesday

7:30 - 9:00 am.....Asilomar Breakfast and  
Box lunch pick-up  
(Asilomar lodgers only)

# ASILOMAR GROUNDS MAP



## MONTEREY BAY AREA ATTRACTIONS

Sunday afternoon is scheduled free time. You are encouraged to relax on your own or with your fellow attendees. **Look for sign-up sheets in the session room** for those interested in group activities. Do you have a car and wish to visit the aquarium? Do you want to rent bikes with others and tour around the area? How about kayaking around Monterey Bay admiring sea otters and the renowned kelp forest as you paddle? Do you want to rent some clubs and play golf? **Be an instigator and list your activity on a sign-up sheet for others to join you.**

### Some Ideas...

Accessible by foot, bus, bike (there are bikes for rent at Asilomar) or by rental car:

- In Monterey - Monterey Bay Aquarium, Fisherman's Wharf, Cannery Row, kayaking on the bay.
- Pebble Beach attractions include the 17-Mile Drive which is accessible free-of-charge on foot or enter by car for a fee.

Accessible by car:

- Carmel Valley is home to many wineries, farms, ranches and the historic Carmel Mission. Hiking in Big Sur or Point Lobos.

At Asilomar:

- Walking trails and self-guided tours throughout the Asilomar campus. Inquire at front desk for details.



Computational methods are ubiquitously used in mass spectrometry, and they have a long history of being applied to all its aspects from data acquisition to data interpretation. These methods include signal processing, search and pattern matching algorithms. Recently the application of machine learning methods to science and society have increased dramatically, and some of these methods have found mass spectrometry applications. At the same time access to large amounts of open publicly available mass spectrometry data has enabled new types of inquiries. This proposed conference will cover the main applications of computational methods to mass spectrometry data.

**We have included ample time for Q&A and interactions between all attendees. We hope you take the opportunity to engage, learn, and have enjoy your time at Asilomar, “the refuge by the sea”.**

*Nuno Bandeira, David Fenyő, and Olga Vitek*  
*Co-Organizers, ASMS Asilomar Conference on Mass Spectrometry*

## FRIDAY, OCTOBER 13, 2023

- 3:00 - 6:00 pm      Name badge pick-up in Chapel
- 3:30 - 5:30 pm      Open to All: **Hands-on Tutorial: David Tabb** (GenNext Technologies)  
**Superior Routes to mzML for Bruker timsTOF and SCIEX TripleTOF in Fast Photochemical Oxidation of Proteins**  
*Files for advance download (before you travel) are strongly recommended. Look for email from [info@asms.org](mailto:info@asms.org) for instructions to download the materials. Please also review the software and machine requirements [HERE](#) to fully participate.*
- 6:00 - 7:00 pm      Asilomar Dinner, Crocker Dining Hall, for Asilomar lodgers.  
*If you are staying offsite and wish to have dinner with the group, purchase separate dinner tickets with your conference registration.*

### 7:15 - 8:15 PM, Chapel OPENING SESSION

- 7:15 - 7:20 pm      Opening Remarks from organizers: Nuno Bandeira, David Fenyő, and Olga Vitek
- 7:20 – 8:00 pm      Olga Vitek presiding  
Keynote Talk: A Christmass Carol - Past, Present and Future Challenges for Computational Proteomics, **Martin Frejno**, MSAID  
*Followed by 5 minutes Q&A*
- 8:05 - 8:10 pm      About the ASMS Asilomar Conference, **Chris Anderton**, ASMS Asilomar Committee
- 8:10 - 8:15 pm      Welcome to the reception presentation; **Zac Anderson**, Bioinformatic Solutions, Inc.

### 8:15 - 9:30 PM, Chapel EVENING RECEPTION sponsored by Bioinformatic Solutions, Inc. & POSTERS

Snacks and drinks are provided at the reception thanks to this evening's reception sponsor, Bioinformatics Solutions, Inc.

*All posters will be displayed for the entire conference. See poster list pages 12-13.*



Bioinformatics Solutions Inc.



# TAKE DISCOVERY TO NEW HEIGHTS WITH DEEP PROTEOMICS SOLUTIONS

## • ABOUT US

Bioinformatics Solutions Inc. (BSI) is a world leading solution provider for mass spectrometry-based proteomics and committed to advancing research with AI-driven biotechnology data analysis solutions. Our mission is to facilitate drug discovery and advance the frontier of biological research through AI-driven commercial software and professional services for discovery proteomics.

## • PROFILE COMPANY

At BSI, we collaborate with leading researchers from the academic, pharmaceutical, and biotechnology sectors, with the aim to provide advanced AI-based solutions to gain comprehensive knowledge in proteomics, immunopeptidomics, and biomedicine research. We believe our strongest asset is our ability to bring the right people together: pioneering scientists, award-winning researchers, technology developers, and AI innovators to execute our mission.

## • WHAT WE DO

BSI is best known in the proteomics research community for the development of the software; PEAKS. PEAKS is used to identify and quantify proteins in very complex biological samples with LC-MS. At BSI, our group is continually involved in research and the advancement of our algorithms to provide solutions to facilitate the understanding of life sciences and are designed to elucidate important biological questions

## ANNOUNCEMENT

*At BSI, we want PEAKS at the forefront of research and extend the deep learning revolution to discovery proteomics, immunopeptidomics, glycoproteomics, and biotherapeutic development. By using innovative approaches in solving optimisation problems by using deep learning and dynamic programming, we hope to push new boundaries of discovery*



PEAKS Studio and PEAKS Online are a complete vendor-neutral solution for discovery proteomics. With DDA and DIA support, PEAKS provides sensitive and very accurate peptide/protein identification and quantification.



PEAKS AB Software provides a powerful, automated solution for the complete de novo sequencing of proteins and in-depth glycan profiling from high-resolution tandem mass spectrometry datasets.



PEAKS GlycanFinder is a comprehensive software for in-depth glycoproteomic analysis with glycan structural resolution. It utilises a glycopeptide-based approach to profile the glycoproteins from LC-MS/MS data.



BSI focuses on proteomic analysis using mass spectrometry and bioinformatics to provide professional CRO services for antibody sequencing, and identification and characterization of proteins and glycans.



## NOTES



## NOTES

## SATURDAY, OCTOBER 14, 2023

7:30 - 9:00 am      Asilomar Breakfast, Crocker Dining Hall, *for Asilomar lodgers only.*

| <b>9:00 AM – 12:00 PM, Chapel</b><br><b>OPEN PROBLEMS IN THE INTERPRETATION OF MS DATA</b><br><i>There is a five-minute gap after each talk for Q&amp;A.</i><br>Sam Payne, presiding |  |
|--|--|
| 9:00 - 9:20 am   | Development of Biologically Aware Instrument Methods; <b>Devin K. Schweppe</b> , <i>University of Washington</i>   |
| 9:25 - 9:45 am   | The Final Frontier: These are the Voyages Through a Latent Space Shared by Mass Spectra and Peptides; <b>Will Fondrie</b> , <i>Talus Bioscience</i>                                      |
| 9:50 - 10:10 am  | The Future is Predicted: Enabling Challenging Proteomics Workflows with Machine Learning; <b>Ralf Gabriels</b> , <i>VIB-UGent Center for Medical Biotechnology</i>                       |
| 10:15- 10:40 am  | Coffee Break   |
| 10:40 - 11:00 am   | Challenges in Processing Omics Multidimensional MS measurements and Opportunities to Address Them Using AI; <b>Aivett Bilbao</b> , <i>Pacific Northwest National Laboratory</i>          |
| 11:05 - 11:25 am   | Interpretation of DIA Data for Human Identification in Forensics; <b>Paul Rudnick</b> , <i>Spectragen Informatics</i>  |
| <b>Short Talks Selected from Submitted Abstracts</b>   |  |
| 11:30 - 11:40 am   | LipidOz: Automated Elucidation of Lipid Double Bond Positions from Ozone-Induced Dissociation Mass Spectrometry Data; <b>Xueyun Zheng</b> , <i>Pacific Northwest National Laboratory</i> |
| 11:45 - 11:55 am   | Computational Problems in Mass Spec Analysis of Nucleic Acids; <b>Marshall W. Bern</b> , <i>Protein Metrics</i>  |

12:00 - 1:00 pm      Asilomar Lunch, Crocker Dining Hall, *for Asilomar lodgers and attendees who pay the offsite fee during online registration.*

*See next page for Saturday afternoon program.*

## SATURDAY, OCTOBER 14, 2023 - *continued*

### 1:15 - 3:10 PM, Chapel DATA SHARING AND REUSE

*There is a five-minute gap after each talk for Q&A.*

Will Fondrie, presiding

|   |   |
|---|---|
| 1:15 - 1:35 pm                                      | Advances and Opportunities in Repository-Scale Mass Spectrometry Data Analysis; <b>Nuno Bandeira</b> , <i>University of California, San Diego</i>   |
| 1:40 - 2:00 pm                                      | Large-Scale Reuse of Proteomics Mass Spectrometry Data with PeptideAtlas; <b>Eric Deutsch</b> , <i>Institute for Systems Biology</i>  |
| 2:05 - 2:25 pm                                      | An Overview of Public Proteomics Data Reuse and Dissemination Activities in PRIDE; <b>Ananth Prakash</b> , <i>EMBL-EBI</i>  |
| 2:30 - 2:50 pm                                      | Accessible, Reproducible, and Sharable Quantitative Single Cell Proteomic Data Analysis with the Platform for Single Cell Science (PSCS); <b>Jesse Meyer</b> , <i>Cedars-Sinai Medical Center</i> |
| <b>Short Talk Selected from Submitted Abstracts</b> |   |
| 2:55 - 3:05 pm                                      | Standardizing Nontargeted Metabolomics and Lipidomics: The LC-BinBase Environment; <b>Oliver Fiehn</b> , <i>University of California, Davis</i>   |

3:10 pm                      Gather outside Chapel for Group Photo (weather permitting)

3:15 - 4:00 pm            Free Time

### 4:00 - 5:30 PM, Chapel SINGLE-CELL

*There is a five-minute gap after each talk for Q&A.*

Jesse Meyer, presiding

|   |  |
|---|--|
| 4:00 - 4:20 pm                                      | Single Cell Asymmetry in Early Embryonic Development; <b>Aleksandra Petelski</b> , <i>Parallel Squared Technology Institute</i>  |
| 4:25 - 4:45 pm                                      | Open Opportunities in Single Cell Proteomics Algorithms; <b>Sam Payne</b> , <i>Brigham Young University</i>  |
| 4:50 - 5:10 pm                                      | Computational Causal Inference Methods and Single Cell Proteomics Enable the Estimation of Interventions from Purely Observational Experiments; <b>Devon Kohler</b> , <i>Northeastern University</i> |
| <b>Short Talk Selected from Submitted Abstracts</b> |  |
| 5:15 - 5:25 pm                                      | How Many Proteins is Enough? The Race for Utility in Single-Cell Proteomics; <b>Alyssa Nitz</b> , <i>Brigham Young University</i>  |

5:30 - 6:00 pm            Free Time

6:00 - 7:00 pm            Asilomar Dinner, Crocker Dining Hall, *for Asilomar lodgers.*  
*If you are staying offsite and wish to have dinner with the group, purchase separate dinner tickets with your conference registration.*

*See next page for Saturday evening program.*

## SATURDAY, OCTOBER 14, 2023 - continued

### 7:15 – 7:45 PM, Chapel POSTER HIGHLIGHT TALKS

Sixteen 90-second lightning-style talks featuring poster presenters.

Nuno Bandeira, David Fenyo, and Olga Vitek, presiding

**Dylan Ross** (Pacific Northwest National Laboratory): *Combined DDA-DIA Lipidomics Data Acquisition and Analysis Workflow* [Poster 20]

**Felix Friedrich** (Uppsala University): *A Data Processing Pipeline for Metabolite Profiling of Individual Cells using nano-DESI MS* [Poster 21]

**Iryna Abramchuk** (University of Ottawa): *Supervised Learning Algorithms for Real-Time Optimization of Mass Spectrometry-Based Proteomics Data Acquisition to Improve Proteome and Interactome Coverage* [Poster 23]

**Olatomiwa Bifarin** (Georgia Institute of Technology): *Automated Machine Learning/Explainable AI (AutoML/XAI) for MS Metabolomics: Improving Cancer Diagnostic Models* [Poster 24]

**Sai Srikanth Lakkimsetty** (Northeastern University): *Unsupervised Co-Registration of Hematoxylin and Eosin (H&E) Stained Microscopy Images and Mass Spectrometry Images (MSI) with Feature Filtering* [Poster 25]

**Arzu Tugce Guler** (Institute for Experiential AI at Northeastern University): *Multiplexing Multiple Digests in MS-Based Proteomics Analysis for Deeper Peptide and Protein Coverage* [Poster 26]

**Nolan McLaughlin** (Washington University in Saint Louis): *Kingfisher Analytical: A New Open Source Comprehensive Statistical HDX-MS Software* [Poster 27]

**Yuanyue Li** (UC Davis): *Flash Entropy Search to Query All Mass Spectral Libraries in Real Time* [Poster 28]

**Zhenru Zhou** (Genentech): *PepMapViz: A Versatile Toolkit for Peptide Mapping, Visualization, and Comparative Exploration* [Poster 28]

**Dirk Walther** (Kymera Therapeutics): *An Integrated Approach to Leveraging Proteomics Data in Targeted Protein Degradation Drug Discovery* [Poster 30]

**Xiaofeng Xie** (Brigham Young University): *MS Connect: Open-Source End-to-End Automation Platform for Mass Spectrometry Data Management, Analysis and Visualization* [Poster 31]

**Rui Xu** (The Ohio State University): *Multiple & Optimal Screening Subset (MOSS): A Method Selecting Global Characteristic Congeners for Robust Food-Omics Analysis* [Poster 32]

**Huaxu Yu** (West Coast Metabolomics Center, University of California, Davis): *Data Alignment of Untargeted LC-MS/MS Experiments Using Internal Standards* [Poster 33]

**William Watson** (Southwest Research Institute): *Suspect Screening of Consumer Products using Machine Learning* [Poster 34]

**Samantha Johnson** (Pacific Northwest National Laboratory): *Towards a Comprehensive Computational Model of Electrospray Ionization in Mass Spectrometry of Acetonitrile-Water-Amino Acid Droplets* [Poster 35]

**WELCOME TO THE RECEPTION** (7:45 - 7:50 pm)

Welcome to the reception presentation; **Heidi Vitrac**, Bruker

7:50 - 9:30 PM, Chapel

### EVENING RECEPTION sponsored by Bruker & POSTERS

Snacks and drinks are provided at the reception thanks to this evening's reception sponsor, Bruker.

All posters will be displayed for the entire conference. See poster list pages 12-13.





# Discover Bruker Mass Spectrometry Software Solutions

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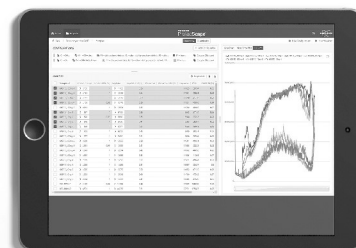
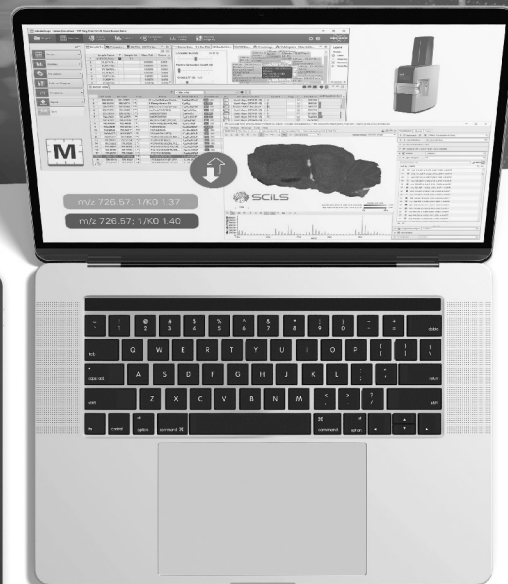
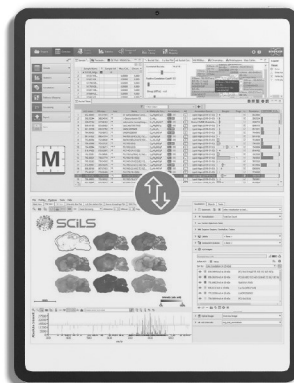
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## REQUEST A DEMO TODAY!



## NOTES

## SUNDAY, OCTOBER 15, 2023

7:30 - 9:00 am Asilomar Breakfast, Crocker Dining Hall, *for Asilomar lodgers only.*

| <b>9:00 AM - 12:00 PM, Chapel</b><br><b>ADVANCES AND CHALLENGES IN MS-BASED QUANTITATION</b><br><i>There is a five-minute gap after each talk for Q&amp;A.</i><br>David Fenyö, presiding |   |
|--|---|
| 9:00 - 9:20 am   | Targeted Approaches to DIA Data Analysis: Extracting Information from Multiplexed MS Spectra; <b>Hannes Röst</b> , University of Toronto            |
| 9:25 - 9:45 am   | Triqler, a Hierarchical Bayesian Model for Protein Summarization; <b>Lukas Kall</b> , SciLifeLab  |
| 9:50 - 10:10 am  | Mass Spectrometry-Based Approaches for Chemoproteomics and Activity-Based Protein profiling; <b>Lindsay Pino</b> , Talus Bioscience                 |
| 10:15 - 10:40 am   | Coffee Break  |
| 10:40 - 11:00 am   | Computational Methods for the Analysis of Thermal Proteome Profiling Data; <b>Frank Stein</b> , EMBL  |
| 11:05 - 11:25 am   | Thermal Proteome Profiling with MSstats; <b>Olga Vitek</b> , Northeastern University  |
| 11:30 - 11:40 am   | Evaluating Proteomics Imputation Methods with Improved Criteria; <b>Lincoln Harris</b> , University of Washington                                   |
| <b>Short Talk Selected from Submitted Abstracts</b>  |   |
| 11:45 - 11:55 am   | New Computational Strategies for Overcoming Analytical Challenges of Emerging Modalities in the Pharmaceutical Industry; <b>Wendy Zhong</b> , Merck |

12:00 - 1:00 pm Asilomar Lunch, Crocker Dining Hall, *for Asilomar lodgers and attendees who pay the offsite fee during online registration.*

1:00 - 6:00 pm **FREE AFTERNOON**

6:00 - 7:00 pm Asilomar Dinner, Crocker Dining Hall, *for Asilomar lodgers.*  
*If you are staying offsite and wish to have dinner with the group, purchase separate dinner tickets with your conference registration.*

*See next page for Sunday evening program.*

**SUNDAY, OCTOBER 15, 2023 - *continued***

**7:15 – 8:00 PM, Chapel**

**Panel Discussion  
PROMISES & PERILS OF MS MACHINE LEARNING**

Moderator: Lindsay Pino

Panelists: Aivett Bilbao, Will Fondrie, Devon Kohler, and Raf Van de Plas

**8:00 - 9:30 PM, Chapel**

**EVENING RECEPTION & POSTERS**

All posters will be displayed for the entire conference. See poster list on pages 12-13.



## MONDAY, OCTOBER 16, 2023

7:30 - 9:00 am Asilomar Breakfast, Crocker Dining Hall, *for Asilomar lodgers only.*

**9:00 - 10:40 AM, Chapel**  
**SPATIAL MASS SPECTOMETRY**  
There is a five-minute gap after each talk for Q&A.

Olga Vitek, presiding

- 9:00 - 9:20 am Bridging timsTOF Data with Open-Source Software Using TIMSCONVERT; **Gordon Luu**, *Bruker*
- 9:25 - 9:45 am What's New in Cardinal for MS Imaging Pre-Processing and Machine Learning; **Kylie Bemis**, *Northeastern University*
- 9:50 - 10:10 am Spatially Driven Biomarker Candidate Discovery by Interpretable Machine Learning of Imaging Mass Spectrometry and Multimodal Imaging Measurements; **Raf Van de Plas**, *Delft University of Technology*
- 10:15 - 10:35 am Building Molecular Atlases of Human Organs from Multimodal Imaging Methods; **Chris Anderton**, *Pacific Northwest National Laboratory*

10:40 - 11:00 am Coffee Break

**11:00 - 11:50 AM, Chapel**  
**BIOLOGICAL AND CLINICAL APPLICATIONS - PART I**  
There is a five-minute gap after each talk for Q&A.

Kelly Ruggles, presiding

- 11:00 - 11:20 am Biomarker Discovery Experiments: From a Model Organism to Clinical Study; **Meena Choi**, *Genentech*
- 11:25 - 11:45 am Evaluation of Analysis Strategies for Data-Independent Acquisition Proteomics Using a Large-Scale Dataset Comprising Inter-Patient Heterogeneity; **Klemens Fröhlich**, *Universität Basel*

12:00 - 1:00 pm Asilomar Lunch, Crocker Dining Hall, *for Asilomar lodgers and attendees who pay the offsite fee during online registration.*

## MONDAY, OCTOBER 16, 2023 - *continued*

1:15 - 2:45 PM, Chapel

### BIOLOGICAL AND CLINICAL APPLICATIONS - PART II

There is a five-minute gap after each talk for Q&A.

Meena Choi, presiding

- 1:15-1:35 pm Translating Cancer Proteogenomics Data into Biological and Clinical Insights; **Bing Zhang**, *Baylor College of Medicine*
- 1:40 - 2:00 pm Using Deep Learning to Integrate Histopathology and Proteogenomics; **David Fenyö**, *NYU Langone Medical Center*
- 2:05 – 2:25 pm Using Multiomic Integration to Understand Cardiovascular Disease, Cancer and Autoimmunity; **Kelly Ruggles**, *NYU Langone Medical Center*
- Short Talk Selected from Submitted Abstracts**
- 2:30 - 2:40 pm A Multi-Modal Computational Image Fusion Workflow Incorporating MALDI Imaging Mass Spectrometry and Microscopy for The Study of Small Pharmaceutical Compounds; **Zhongling Liang**, *University of Florida*

2:45 - 3:15 pm Coffee Break

3:15 – 4:00 PM, Chapel

### KEYNOTE TALK

Followed by five minutes for Q&A

Nuno Bandeira, presiding

- 3:15-3:55 pm Repository Scale Discovery of Previously Undescribed Microbial Disease-Associated Metabolites and Pathways in Human Biology; **Pieter Dorrestein**, *University of California, San Diego*

4:00 - 6:00 pm FREE TIME

6:00 - 7:00 pm Asilomar Dinner, Crocker Dining Hall, *for Asilomar lodgers*.

7:15 - 8:00 PM, Chapel

### Panel Discussion

#### THE FUTURE OF COMPUTATIONAL MASS SPECTROMETRY

Moderator: David Fenyö

Panelists: Kylie Bemis, Pieter Dorrestein, Oliver Fiehn, Martin Frejno, and Lindsay Pino

8:05 - 9:30 PM, Fire Pit below Crocker Dining Hall

### BONFIRE & S'MORES

If you are not familiar with a 'S'more' (graham crackers, chocolate bar, and toasted marshmallow) you will learn!

It's sticky and delicious!

*Last call for bar is 9:15 pm.*

## TUESDAY, OCTOBER 17, 2023

7:30 - 9:00 am Asilomar Breakfast, Crocker Dining Hall, *for Asilomar lodgers only*.

## POSTER LIST

All posters will be displayed for the entire conference. Poster presenters will present during the evening receptions on Friday, Saturday, and Sunday.

- Poster 1 Integrated Omics for Precision Emergency Medicine after Traumatic Injury; **Ian LaCroix**, *University of Colorado Anschutz*
- Poster 2 Metabolomic Profile Characterization of Tissue Adjacent to Tumor for Improved Cancer Prediction and Determination of Surgical Margins; **Faith Jackobs**, *Baylor College of Medicine*
- Poster 3 FragPipe Enhancements: Integrating MSFragger-DIA and MSFragger-WWA for Advanced Single-Cell and Bulk-Cell Proteomics Analysis; **Fengchao Yu**, *University of Michigan*
- Poster 4 *Identifying Colocalized Compounds in Mass Spectrometry Images of Diverse Tissue Samples Using Unsupervised Deep Learning*; **Emerson Hernly**, *Purdue University*
- Poster 5 Absolute Quantitation of Metabolites Using Machine Learning and “Standard Candles” as Universal Calibrators - the Third Generation Model; **Tian Cai**, *MatterWorks*
- Poster 6 Real-Time de novo Sequencing of Peptide Antigens using ProteoScape™ for “Run and Done” 4D-Immunopeptidomics; **Heidi Vitrac**, *Bruker Scientific LLC*
- Poster 7 Systematic Evaluation and Optimization of PRM Assays for the Quantification of Very Low Abundant Proteins Within Complex Samples; **Christian Schori**, *University of Basel*
- Poster 8 Statistical Methods for Handling Cellular Heterogeneity in Quantitative scMS Experiments: Review Simulations and Recommendations; **Hannah Boekweg**, *Brigham Young University*
- Poster 9 DIA Benchmarking for Biomarker Discovery in Mouse Plasma Using a Complex Proteomic Standard; **Aron Phong**, *Alkahest Inc*
- Poster 10 Development of a MALDI-tims-QTOF Assay for Enhanced Directed Evolution Screening; **Robert Shepherd**, *UC Santa Cruz*
- Poster 11 Integrated Data Service Ecosystem for Mass Spectrometry; **Yuri Corilo**, *Pacific Northwest National Laboratory*
- Poster 12 A Novel Computational Pipeline for Immunopeptidomics with LC-MS; **Baozhen Shan**, *Bioinformatics Solutions Inc.*
- Poster 13 The Quantification of Isotope Enrichment from Two Mass Isotopomers Helps to Reduce the Proteome Complexity in Protein Turnover Estimations; **Rovshan Sadygov**, *University of Texas Medical Branch*
- Poster 14 Multi-omic Landscape Of Squamous Cell Lung Cancer; **Paul Stewart**, *Moffitt Cancer Center*
- Poster 15 Optimizing Peptide Ion Selection and Fragmentation through Real-Time Machine Learning Analysis of Mass Spectrometry Data; **Mathieu Lavallée-Adam**, *University of Ottawa*
- Poster 16: Creation of CID-MS/MS Spectra Using ab initio Molecular Dynamics; **Tobias Kind**, *Enveda Biosciences*
- Poster 17 A New Computational Approach for Multiple Charge Deconvolution; **Yongdong Wang**, *Cerno Bioscience*
- Poster 18 Sage: an Open-Source Tool for Fast -Proteomics Searching and Quantification at Scale; **Michael Lazear**, *Belharra Therapeutics*

## POSTER LIST

All posters will be displayed for the entire conference. Poster presenters will present during the evening receptions on Friday, Saturday, and Sunday.

- Poster 19 Unexpected Challenges in Computational Studies of Larger Gas-Phase Ions Using Electron Structure Methods; **Frantisek Turecek**, *University of Washington*
- Poster 20 Combined DDA-DIA Lipidomics Data Acquisition and Analysis Workflow; **Dylan Ross**, *Pacific Northwest National Laboratory*
- Poster 21 A Data Processing Pipeline for Metabolite Profiling of Individual Cells using nano-DESI MS; **Felix Friedrich**, *Dept. of Chemistry-BMC, Uppsala University*
- Poster 23 Supervised Learning Algorithms for Real-Time Optimization of Mass Spectrometry-Based Proteomics Data Acquisition to Improve Proteome and Interactome Coverage; **Iryna Abramchuk**, *University of Ottawa*
- Poster 24 Automated Machine Learning/Explainable AI (AutoML/XAI) for MS Metabolomics: Improving Cancer Diagnostic Models; **Olatomiwa Bifarin**, *Georgia Institute of Technology*
- Poster 25 Unsupervised Co-Registration of Hematoxylin and Eosin (H&E) Stained Microscopy Images and Mass Spectrometry Images (MSI) with Feature Filtering; **Sai Srikanth Lakkimsetty**, *Northeastern University*
- Poster 26 Multiplexing Multiple Digests in MS-Based Proteomics Analysis for Deeper Peptide and Protein Coverage; **Arzu Tugce Guler**, *Institute for Experiential AI at Northeastern University*
- Poster 27 Kingfisher Analytical: A New Open Source Comprehensive Statistical HDX-MS Software; **Nolan McLaughlin**, *Washington University in Saint Louis*
- Poster 28 Flash Entropy Search to Query All Mass Spectral Libraries in Real Time; **Yuanyue Li**, *University of California, Davis*
- Poster 29 PepMapViz: A Versatile Toolkit for Peptide Mapping, Visualization, and Comparative Exploration; **Zhenru Zhou**, *Genentech*
- Poster 30 An Integrated Approach to Leveraging Proteomics Data in Targeted Protein Degradation Drug Discovery; **Dirk Walther**, *Kymera Therapeutics*
- Poster 31 MS Connect: Open-Source End-to-End Automation Platform for Mass Spectrometry Data Management, Analysis and Visualization; **Xiaofeng Xie**, *Brigham Young University*
- Poster 32 Multiple & Optimal Screening Subset (MOSS): A method Selecting Global Characteristic Congeners for Robust Food-Omics Analysis; **Rui Xu**, *The Ohio State University*
- Poster 33 Data Alignment of Untargeted LC-MS/MS Experiments Using Internal Standards; **Huaxu Yu**, *West Coast Metabolomics Center, University of California, Davis*
- Poster 34 Suspect Screening of Consumer Products using Machine Learning; **William Watson**, *Southwest Research Institute*
- Poster 35 Towards a Comprehensive Computational Model of Electrospray Ionization in Mass Spectrometry of Acetonitrile-Water-Amino Acid Droplets; **Samantha Johnson**, *Pacific Northwest National Laboratory*



## FUTURE EVENTS

November/December 2023

### Online Short Courses

Untargeted Metabolomics: From Basic Methods to Adv. Workflows and Isotope Labeling  
Two-day Course: November 30 & December 1

High Resolution Mass Spectrometry for Qualitative and Quantitative Analysis: An Introduction  
Two-day Course: December 7 & 8

LC-MS/MS: Techniques using Electrospray, APCI and APPI  
Two-day Course: December 14 & 15

More Information at <https://www.asms.org/conferences/online-short-courses>

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January 21 - 24, 2024

### **34th Sanibel Conference on Mass Spectrometry for Complex Mixtures in Energy and the Environment**

Hilton St. Petersburg Bayfront | St. Petersburg, Florida

*Organizers*

Janne Janis (University of Eastern Finland), and Julian Whitelegge (UCLA)

More information at <https://www.asms.org/conferences/sanibel-conference>

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June 4 – 8, 2024

### **72nd ASMS Conference on Mass Spectrometry and Allied Topics**

Anaheim Convention Center | Anaheim, California

**Abstract Deadline is February 2, 2024**

More information at <https://www.asms.org/conferences/annual-conference>