



# Conference on Ion Chemistry and Mass Spectrometry

## Schedule of Presentations

January 13–15, 2023

UCLA Conference Center, Lake Arrowhead, CA

### FRIDAY, JANUARY 13

3:30 PM CHECK-IN AND ROOM ASSIGNMENTS

5:00 – 6:30 PM SOCIAL HOUR

**POSTER PRESENTERS:** Please put your poster up during the welcome social.

6:30 – 8:00 PM DINNER

### SESSION I      **Presider: Nathan Dalleska**

**8:00 - 8:25** “Quantitative Evaluation of Computationally Derived Therapeutic Inhibitors of TDP-43 307–319 Oligomerization”, **Xikun Liu**, Shuya Duan, Yingying Jin, Ziying Chen, Kristi Lazar Cantrell, Steven K. Burrato, Ambuj K. Singh and Michael T. Bowers,\* *University of California, Santa Barbara, CA*.

**8:25 – 8:50** “Cerium (Ce) Oxide, Carbide, Dioxide, and Carbonyl Cation Bond Energies and the Evaluation of the Exothermic  $\text{Ce} + \text{O} \rightarrow \text{CeO}^+ + e^-$  Chemi-ionization”, **Talley Fenn**, Brandon C. Stevenson, Sara Rockow, and Peter B. Armentrout,\* *University of Utah, Salt Lake City, UT*.

**FRIDAY, JANUARY 13****9:00 – 12:00 PM POSTER SESSION, DRINKS, AND DISCUSSION****POSTER PRESENTATIONS**

1. “Amyotrophic Lateral Sclerosis-associated Mutants of SOD1 Modulate miRNA Biogenesis through Aberrant Interactions with Exportin 5”, **Xingyuan Chen**, Xiaomei He, Yen-Yu Yang, and Yinsheng Wang,\* *University of California, Riverside, CA.*
2. “Bridging Ion Mobility Mass Spectrometry and Atomic Force Microscopy: A Study of TDP43 Aggregation”, **Dorothea Duan**, Xikun Liu, Yingying Jin, Steven K. Burrato, Ambuj K. Singh, and Michael T. Bowers,\* *University of California, Santa Barbara, CA.*
3. “Coaggregation and Oligomeric Assembly of HIV1-TAT (47–57) and Amyloid Beta (25–35)”, **Dmitriy Prokopovich** and Michael T. Bowers,\* *University of California, Santa Barbara, CA.*
4. “IRMPD Spectroscopy of Biomimetic Complexes: Metallated Histidine Dipeptide”, **Brandon C. Stevenson**, Giel Berden, Jonathan Martens, Jos Oomens, and P. B. Armentrout,\* *University of Utah, Salt Lake City, UT.*
5. “Gas-Phase Intramolecular Photo Crosslinking in Tetrazole-Peptide Conjugates”, **Jiahao Wan**, Haocheng Qian, and František Tureček,\* *University of Washington, Seattle, WA.*
6. “Binding Energies of Hydrated Calcium Hydroxide Ion Complexes: A Guided Ion Beam and Theoretical Investigation”, **Fan Yang** and Peter B. Armentrout\*, *University of Utah, Salt Lake City, UT.*
7. “Carbene Crosslinking in Gas-Phase Peptide Ion Scaffolds”, **Hongyi Zhu**, Václav Zima, Emily Ding, and František Tureček,\* *University of Washington, Seattle, WA.*
8. “Aggregation Study of Alpha-Synuclein Using IM-MS”, **Zhiyuan Zhu** and Michael T. Bowers,\* *University of California, Santa Barbara, CA.*
9. “Tracking Isomerizations in Adenine and 9-Methyladenine High-Energy Cation Radicals by UV-Vis Photodissociation Action Spectroscopy”, **Vaclav Zima**, Mikulas Vik, Jiahao Wan, Josef Cvacka, and František Tureček,\* *University of Washington, Seattle, WA.*
10. “Applying Internal Fragments for Top-Down Mass Spectrometry of Intact Monoclonal Antibodies and Antibody-Drug Conjugates”, **Benquan Wei**, Carter Lantz, Weijing Liu, Rosa Viner, Rachel R. Ogorzalek Loo, Iain D. G. Campuzano, and Joseph A. Loo,\* *University of California, Los Angeles, CA.*

**FRIDAY, JANUARY 13****9:00 – 12:00 PM POSTER SESSION, DRINKS, AND DISCUSSION****POSTER PRESENTATIONS (continued)**

11. “Exploring the Proximity Proteomes of YY1 by APEX Labeling”, **Zhongwen Cao** and Yinsheng Wang,\* *University of California, Riverside, CA.*
12. “Novel Free Radical and Fluorescent Tag(Gly•RadiFluor) for Simultaneous Glycan Quantitation and Characterization via UPLC-Orbitrap MS”, Rayan Murtada, Shane Fionn, Teuta Hida, and **Jinshan Gao**,\* *Montclair State University, Montclair, NJ.*
13. “Pinpointing Isomerized Residue Location in Peptides with MS<sup>3</sup> Analysis”, **Hoi Ting Wu** and Ryan R. Julian,\* *University of California, Riverside, CA.*
14. “Solvent Influence on the Acidity of Organic Compounds and Small Peptides”, **Kim Harvey**, Erica Meng, Raj Patel, Mandy Brinkmann, Michael Browne, and Jianhua Ren,\* *University of the Pacific, Stockton, CA.*
15. “Computational Studies of the Gas-Phase Acidity of D/L-Cysteine-Containing Tetrapeptides”, **Shiyuan Wang**, Yuntao Zhang, and Jianhua Ren,\* *University of the Pacific, Stockton, CA.*
16. “Fragmentation Patterns of Peptoids Containing a Basic Residue”, **Ashleigh Ramos**, Yadwinder Singh Mann, and Jianhua Ren,\* *University of the Pacific, Stockton, CA.*
17. “Deciphering the Relationship Between Gut Microbe-Derived SCFAs and Dietary Carbohydrates Using Rapid-Throughput LC-MS Based Platforms”, **Cheng-Yu Weng**, Christopher Suarez, Garret Couture, Chad Masarweh, Karen Kalanetra, David Mills, and Carlito B. Lebrilla,\* *University of California, Davis, CA.*
18. “Using Native Top-Down MS to Structurally Characterize Carbonic Anhydrase Bound to Inhibitors”, **Eileen J. Olivares** and Joseph A. Loo,\* *University of California, Los Angeles, CA.*
19. “High-throughput Automated Sample Preparation for Human Milk Oligosaccharides Analysis”, **Aaron Stacy** and Carlito B. Lebrilla”,\* *University of California, Davis, CA.*
20. “*i*-Motif Stabilization Using Cytosine Derivatives”, **Dezere Gil**, **Michael Sahagun**, and Hou Ung,\* *University of La Verne, La Verne, CA.*

**FRIDAY, JANUARY 13****9:00 – 12:00 PM POSTER SESSION, DRINKS, AND DISCUSSION****POSTER PRESENTATIONS (continued)**

21. “Statistical Analysis for Top-Down MS Data”, **Thomas A. Shoff** and Ryan R. Julian,\* *University of California, Riverside, CA.*
22. “Glycoproteomics Analysis of High-Density Lipoproteins in Alzheimer’s Disease Patients”, **Armin Oloumi**, Brian Hong, Yasmine Bouchibti, Jennyfer Tena, Angela Zivkovic, and Carlito B. Lebrilla,\* *University of California, Davis, CA.*
23. “5-Aza Substitution Weakens the Glycosidic Bond Stability of 2'-Deoxycytidine: Investigations via ER-CID Experiments and Theoretical Calculations”, **Christopher Federlein**, Ezekiel Israel, and M. T. Rodgers,\* *Wayne State University, Detroit, MI.*
24. “Incorporation of <sup>13</sup>C-Monosaccharides in Glycoproteins Analyzed Using Orbitrap LC-MS/MS Glycoproteomics”, **Michael Russelle Alvarez**, Armin Oloumi, Sheryl Joyce Grijaldo, and Carlito B. Lebrilla,\* *University of California, Davis, CA.*
25. “Hydroquinone Modification of Free Thiols Allows for Site-Selective Radical Chemistry in Peptides and Proteins”, **Evan E. Hubbard** and Ryan R. Julian,\* *University of California, Riverside, CA.*
26. “Single-Cell Proteomic Analysis of Drosophila Oocytes”, **Merin Rixen**, Joseph A. Loo,\* and Rachel Loo,\* *University of California, Los Angeles, CA.*
27. “Spontaneous Chemical Modifications Identified in Human Tau Samples”, **Brielle L. Van Orman** and Ryan R. Julian,\* *University of California, Riverside, CA.*
28. “Structural Glycosphingolipid Fragmentation using CID with nano-HPLC-MS/MS”, **Ryan Schindler** and Carlito B. Lebrilla,\* *University of California, Davis, CA.*
29. “Electron Capture Dissociation on a Cyclic Ion Mobility Enabled Q-ToF Mass Spectrometer Provides Higher Structural Resolution in HDX-MS Experiments”, **Si Cheng**,<sup>2</sup> Owen Cornwell,<sup>1</sup> Ying Qing Yu,<sup>2</sup> Bobette Frye,<sup>2</sup> Dale-Cooper-Shepherd,<sup>1</sup> Nicola Johnston,<sup>1</sup> Jonathan Fox,<sup>1</sup> and Malcolm Anderson,<sup>1</sup> *Waters Corporation, <sup>1</sup>Wilmslow, UK and <sup>2</sup>Milford, MA.*

**SATURDAY, JANUARY 13**

**8:00 – 9:00            BREAKFAST**

**SESSION II            Presider: Hao Chen**

**9:00 – 9:25**            “METTL3 Promotes Histone H3K9 Acetylation through Recruitment of Histone Acetyltransferase 1 to Chromatin”, **Yen-Yu Yang**, Xiaomei He, Jun Yuan, Chengjie Ma, and Yinsheng Wang\*, *University of California, Riverside, CA*.

**9:25 – 9:50**            “Phosphate Fingerprints Reveal Binding Sites between Proteins and Ligands by Native Top-Down Mass Spectrometry”, **Jessie Le**, Rachel R. Ogorzalek Loo, and Joseph A. Loo,\* *University of California, Los Angeles, CA*.

**9:50 – 10:15**            “Investigation of b-Ion Formation Using Glycine Polymers”, **Evan H. Perez**, Brandon Stevenson, Ahmed Mohammed, Franziska Dahlmann, Michael Van Stipdonk, Mark A. Johnson, and Peter B. Armentrout,\* *University of Utah, Salt Lake City, UT*.

**10:15 – 10:45            BREAK**

**10:45 – 11:10**            “Activation and Relaxation of Protein Ions Observed Using Time-Resolved Ion-Neutral Collision Cross Sections in an FT-ICR MS”, **Savannah R. Porter**, Noah J. Mismash, Andrew J. Arslanian, and David V. Dearden,\* *Brigham Young University, Provo, UT*.

**11:10 – 11:35**            “Quantitative Analysis of Anticancer Drugs in Single Multicellular Spheroids”, **Zongkai Peng**, Yunpeng Lan, and Zhibo Yang,\* *University of Oklahoma, Norman, OK*.

**11:35 – 12:00**            “Gold-Catalyzed Arylation of Free Thiols for 266 nm Photodissociation”, **Jacob W. Silzel**, Phil Farias, Hill Harman, and Ryan R. Julian, \* *University of California, Riverside, CA*.

**12:00 – 3:00            LUNCH AND FREE TIME**

**SATURDAY, JANUARY 14**

**3:00 – 3:10            CONFERENCE PHOTO**

**PLEASE MEET IN FRONT OF CONFERENCE CENTER PROMPTLY AT 3:00 PM TO ENSURE THAT EVERYONE IS INCLUDED IN THE CONFERENCE PHOTO !!!**

**SESSION III        Presider: Ryan Julian**

**3:20– 3:45**        “Progress on Glycomic and Glycoproteomic Analyses”, **Carlito Lebrilla**,\* *University of California, Davis, CA.*

**3:45 – 4:10**        “Small GTPases in Radioresistance of Breast Cancer Cells”, **Zi Gao** and Yinsheng Wang,\* *University of California, Riverside, CA.*

**4:10 – 4:35**        “Combined AFM and IM-MS Method on Studying the Early Aggregation Pathway of a Model Peptide from Alpha Synuclein Non-Amyloid-Core (NAC) Region — 68GAVVTGVTAVA78 ”, **Yingying Jin**, Zhiyuan Zhu, Steve Buratto, and Michael T. Bowers,\* *University of California, Santa Barbara, CA.*

**4:35 – 5:05            BREAK**

**5:05 – 5:30**        Utilizing Hydrogen-Deuterium Exchange to Induce Mass Distribution Shifts in Cyclic Ion Mobility Spectrometry”, **David L. Williamson**, Tyson K. Trimble, and Gabe Nagy,\* *University of Utah, Salt Lake City, UT.*

**5:30 – 5:55**        “Time-Resolved Collision Cross Section Measurements for Gas-Phase Host-Guest Complexes”, **Noah J. Mismash**, Savannah R. Porter, Tanner R. Taylor, Bryce J. Davis, Andrew J. Arslanian, and David V. Dearden,\* *Brigham Young University, Provo, UT.*

**5:55 – 6:20**        “MassLite: Integrated MS Data Treatment Platform with Advanced Alignment Algorithm”, **Zhu Zou** and Zhibo Yang,\* *University of Oklahoma, Norman, OK.*

**6:30 – 8:00            DINNER**

**SATURDAY, JANUARY 14**

**8:00 – 9:30      SATURDAY EVENING LECTURE**

**Presiding: Mary T. Rodgers**

**Celebrating**  
**50<sup>+</sup> Years**  
**of the**  
**Lake Arrowhead Conference**  
**on**  
**Ion Chemistry and Mass**  
**Spectrometry**

**Support for the Saturday evening celebration generously provided by Bruker Daltonics,  
American Elements, and the Waters Corporation.**



**9:30 – 12:00**

**PARTY**

**SUNDAY, JANUARY 15**

**8:00 – 9:00            BREAKFAST**

**SESSION IV            Presider:    Thomas Wyttenbach**

**9:00 – 9:25**            “Microdroplet Digestion of Antibody Proteins”, Pengyi Zhao, Yongling Ai, Harsha P. Gunawardena, Xiaoqin Zhog, Richard N. Zare, and **Hao Chen**,\* *New Jersey Institute of Technology, University Heights Newark, NJ.*

**9:25 – 9:50**            “Spin-Forbidden Lanthanide Cation Reactions with N<sub>2</sub>O: A Guided Ion Beam and Computational Investigation”, **David Loertscher**, Brandon C. Stevenson, and Peter B. Armentrout,\* *University of Utah, Salt Lake City, UT.*

**9:50 – 10:15**            “The Influence of Modifications on the Mechanisms and Energetics for N-Glycosidic Bond Cleavage of Protonated Cytidine Nucleoside Analogues: Tandem Mass Spectrometry and Computational Investigations”, **Ezekiel Israel** and Mary T. Rodgers,\* *Wayne State University, Detroit, MI.*

**10:15 – 11:00 BREAK**

**PLEASE CHECK OUT AND RETURN YOUR KEY DURING THE BREAK; CHECK OUT TIME IS 11:00.**

**11:00 – 11:25**            “Characterization of Glycogen through Glycomic Methods”, **Yasmine Bouchibti**, Cathy Chen, and Carlito B. Lebrilla,\* *University of California, Davis, CA.*

**11:25 – 11:50**            “Native Top-Down Mass Spectrometry of Protein Complexes with Electron Capture Dissociation on a Q-Exactive Ultra-High Mass Range Quadrupole-Orbitrap Mass Spectrometry”, **Boyu Zhao** Carter Lantz, Benqian Wei, Rachel Loo, and Joseph A. Loo,\* *University of California, Los Angeles, CA.*

**12:00 – 1:00                    LUNCH AND DEPART**



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