



Conference on Ion Chemistry and Mass Spectrometry

2009 Conference on Ion Chemistry and Mass Spectrometry
January 16–18, 2009
UCLA Conference Center, Lake Arrowhead, California

SCHEDULE OF PRESENTATIONS

Friday, January 16

3:30 PM CHECK-IN AND ROOM ASSIGNMENTS

5:30 – 6:30 SOCIAL HOUR

Poster presenters, please put your poster up during the welcome social.

6:30 - 7:30 DINNER

SESSION I Presider: Manuel Manard

7:45 - 8:10 “Design of a New High Resolution Ion Mobility Mass Spectrometer and Application to Enkephalin Dimer Formation”, **Nicholas Dupuis**, Paul Kemper, Christian Bleiholder and Michael T. Bowers*, *University of California, Santa Barbara, CA*.

8:10 - 8:35 “Using Gas-Phase Ion Chemistry to Investigate Absolute Reduction Potentials and Electron Solvation in Aqueous Solution”, **William A. Donald**, Ryan D. Leib, Maria Demireva, M. Jeanette Aiken, and Evan R. Williams*, *University of California, Berkeley, CA*.

8:35 – 9:00 “Probing the Mechanism of Electron Capture and Electron Transfer Dissociation with Hydrogen Atom Scavengers and Tags with Variable Electron Affinity”, **Chang Ho Sohn**, Cheol K. Chung, Sheng Yin, Prasanna Ramachandran, Ivory Peng, Joseph A. Loo, and J. L. Beauchamp*, *California Institute of Technology, Pasadena, CA*.

9:00 – 11:00

POSTER SESSION, DRINKS, AND DISCUSSION**POSTER PRESENTATIONS**

1. "High-Throughput, High-Sensitivity Proteomics Platform for Improved Biomarker Discovery and Verification", **Erin S. Baker**, Eric A. Livesay, Daniel J. Orton, William F. Danielson III, David C. Prior, Yehia M. Ibrahim, Ronald J. Moore, Keqi Tang, Ryan T. Kelly, Gordon A. Anderson, Mikhail E. Belov, and Richard D. Smith*, *Pacific Northwest National Laboratory, Richland, WA.*
2. "Infrared Multiphoton Dissociation Action Spectroscopy of DNA Mononucleotides: Effects of Cationization on Gas Phase Conformation", **Yuan-wei Nei**, Nuwan Hallowita, Jeffrey D. Steill, Jos Oomens, and Mary T. Rodgers*, *Wayne State University, Detroit, MI.*
3. "Structures and Binding Energies of Noncovalent Complexes of Peptidomimetic Protonated Nitrogen Bases with 18-Crown-6", Yu Chen and **Mary T. Rodgers***, *Wayne State University, Detroit, MI.*
4. "Manipulating Small Droplets with Pulsed Electric Fields to Examine the Physical Properties and Chemical Reactivity of Gas-Liquid Interfaces", **Evan L. Neidholdt** and J. L. Beauchamp*, *California Institute of Technology, Pasadena, CA.*
5. "Surface-Induced Dissociation of Odd-Electron Peptide Ions", **Julia Laskin***, Zhibo Yang, Corey lam, and Ivan K. Chu, *Pacific Northwest National Laboratory, Richland, WA.*
6. "Tandem MS/MS Investigation of Positively and Negatively Charged Ions Generated by ESI from Tholin Samples: An Implication to Titan's Atmospheric Chemistry", **Arpad Somogyi**, Roland Thissen, Veronique Vuitton, and Mark Smith*, *University of Arizona, Tucson, AZ*
7. "Observing Radical Migration in Peptides Using Photodissociation and Ion-Molecule Reactions", **Ben Moore**, Ryan Julian*, Stephen Blanksby, and Tony Ly, *University of California, Riverside.*
8. "Conformational Effects of Small Molecule Binding to Alpha-Synuclein and its Disease-Related A30P and A53T Mutants", **Anna Erickson**, Megan Grabenauer, Thomas Wyttenbach, Jay R. Winkler, Harry B. Gray, and Michael Bowers* *University of California, Santa Barbara, CA.*
9. "Affinity Capture Mass Spectrometry: A Diagnostic for Bacterial Contamination", **Erin M. Johnson**, Walther Ellis, Donna Wolk, and Vicki H. Wysocki*, *University of Arizona, Tucson, AZ.*
10. "Native Mass Spectrometry as a Structural Probe for Soluble Guanylyl Cyclase", **Anne E. Blackwell** and Vicki H. Wysocki*, *University of Arizona, Tucson, AZ.*
11. "Electron Affinities of Chlorinated Hydrocarbons and Their Electron Capture Structures", **L.D. Betowski***, Mark Enlow, and D.H. Aue, *U. S. Environmental Protection Agency, Las Vegas, NV.*
12. "Using Intensity in Peptide Identification Algorithms", **Wenzhou Li**, Jonathan Goya, and Vicki Wysocki*, *University of Arizona, Tucson, AZ.*
13. "Mass-Balanced H/D-Isotope Dipeptide Tags for Simultaneous Peptide Sequencing and Protein Quantitation", Jongcheol Seo, Min-Soo Suh, Hye-Joo Yoon and **Seung Koo Shin***, *Pohang University of Science and Technology, Pohang, South Korea.*

POSTER PRESENTATIONS (continued)

14. "Mapping Iodination Sites in Whole Proteins by MALDI-MS for Potential Exploration of Solution Phase Protein Structure", **Qingyu Sun** and Ryan R. Julian*, *University of California, Riverside, CA.*
15. "Reactions of Alpha Nucleophiles with Alkyl Halides", Stephanie M. Villano, Nicole Eyet, W. Carl Lineberger, and **Veronica M. Bierbaum***, *University of Colorado, Boulder, CO.*
16. "Structures of Potassiated Aminocarboxylic Acids and Proline Derivatives by IMS/MS", **Bing Gao**, Thomas Wyttenbach, Miriam K. Drayss, Mathias Schäfe, and Michael T. Bowers*, *University of California, Santa Barbara, CA*
17. "Where Does the Electron Go in Peptide Cation-Radicals?", **Frantisek Turecek***, Changtong Hao, and Eva Fung, *University of Washington, Seattle, WA.*
18. "Cross Sectional Areas by Fourier Transform Ion Cyclotron resonance (CRAFTI): A New Method for Probing Ion Conformation", Fan Yang, Jacob Voelkel, and **David V. Dearden***, *Brigham Young University, Provo, UT.*
19. "Mass Spectrometric Characterization of Monorhamnolipid Produced from *P. Aeruginosa* ATCC 9027 Complexes with Pb²⁺ and UO₂²⁺", **Tracey A. Veres**, Arpad Somogyi, and Jeanne E. Pemberton*, *University of Arizona, Tucson, AZ.*

Saturday, January 17

8:00 – 8:30 BREAKFAST

SESSION II Presider: David V. Dearden

8:30 – 8:55 “Wet Grease: Hydration of Hydrophobic Groups Investigated with Infrared Photodissociation Spectroscopy and Theory”, **James S. Prell** and Evan R. Williams*, *University of California, Berkeley, CA.*

8:55 - 9:20 “IRMPD Spectroscopy of Sodiated and Protonated Diethyl and Triethyl Phosphate Esters”, **B. Scott Fales**, Nathaniel O. Fujamade, Chunhai Ruan, Jos Oomens, and M. T. Rodgers*, *Wayne State University, Detroit, MI.*

9:20 – 9:45 “Detecting Phosphorylation the Radical Way”, **Jolene K. Diedrich** and Ryan R. Julian*, *University of California, Riverside, CA.*

9:45 – 10:10 “Vibrational Spectroscopy of $\text{Fe}^+(\text{CH}_4)_n$ ”, **Murat Citir** and Ricardo B. Metz*, *University of Massachusetts, Amherst, MA.*

10:10 – 10:25 BREAK

10:25 – 10:50 “The Effect of Calcium Ions and Peptide Ligands on the Stability of the Calmodulin Dumbbell Structure”, **Thomas Wyttenbach**, Megan Grabenauer, Konstantinos Thalassinos, James H. Scrivens, and Michael T. Bowers*, *University of California, Santa Barbara, CA.*

10:50 – 11:15 “The Development of Retrosynthetic Glycan Libraries to Profile and Classify the Human Serum N-Linked Glycome”, **Scott R. Kronewitter**, Hyun Joo An, Maria Lorna de Leoz, and Carlito B. Lebrilla*, *University of California, Davis, CA.*

11:15 – 11:40 “Ionic Reactions in Desorption Electrospray Ionization Mass Spectrometry”, **Hao Chen**,* Zhixin Jessie Miao, and Yun Winnie Zhang, *Ohio University, Athens, OH.*

11:40 – 12:05 “The Binding Parameter Model: A Quantitative Elucidation of the Fundamental Interactions that Determine the Strength and Specificity of Cation- π Interactions”, **Nuwan Hallowita**, Ravi Amunugama, Chunhai Ruan, Esitima Udonkang, Cliff Frieler, and M. T. Rodgers*, *Wayne State University, Detroit, MI.*

12:05 – 2:10 LUNCH AND FREE TIME

2:10 – 2:30 CONFERENCE PHOTO

SESSION III Presider: Nathan Dalleska

2:30 – 2:55 “Ab Initio Protein Folding Probed by All-Atom Molecular Dynamic Simulations with Replica Exchange Method”, **Chun Wu**, Nicholas F. Dupuis, Joan-Emma Shea, and Michael T. Bowers*, *University of California, Santa Barbara, CA.*

2:55 - 3:20 “All Roads Lead to Rome: Radical Migration Towards the Beta-Carbon Yields Dissociation of the Peptide Backbone at Tyrosine”, **Tony Ly** and Ryan R. Julian*, *University of California, Riverside, CA.*

3:20 – 3:45 “N-linked and Free Oligosaccharide Content of Human Milk”, **John Froehlich**, Eric Dodds, Richard Seipert, Larry Lerno, Mariana Barboza, and Carlito B. Lebrilla*, *University of California, Davis, CA.*

3:45 - 4:10 “The Photoelectron Spectrum of CCl_2^- : The Convergence of Theory and Experiment After a Decade of Debate”, **Scott W. Wren**, Kristen M. Vogelhuber, Kent M. Ervin, and W. Carl Lineberger*, *University of Colorado, Boulder, CO.*

4:10 – 4:30 BREAK

4:30 – 4:55 “Discovery of Glycomic Markers for Cancer”, **Maria Lorna A. de Leoz**, Scott Kronewitter, Hyun Joo An, Jaehan Kim, Ruth Vinall, Suzanne Miyamoto, Larry Young, Ralph de Vere White, Kit S. Lam, and Carlito Lebrilla*, *University of California, Davis, CA.*

4:55 – 5:20 “Investigating Low Barrier Hydrogen Bonds in Linear and Cyclic Diamines”, **Sevana Khodagholian** and Thomas Morton*, *University of California, Riverside, CA.*

5:20 – 5:45 “The Effects of Rapid Analyte/Solvent Mixing for ESI MS of Peptides and Proteins”, **Ivory Peng**, Rachel Loo, and Joe Loo*, *University of California, Los Angeles, CA.*

5:45–6:10 “Formation and Growth of Complex Organics by Gas Phase and Intracluster Reactions”, Paul O. Momoh, Abdel-Rahman Soliman and **M. Samy El-Shall*** *Virginia Commonwealth University, Richmond, VA.*

6:30 - 8:00 DINNER

8:00 - 9:00 ? SATURDAY EVENING

Presider: Erin S. Baker

Symposium and Celebration in Honor of



Michael T. Bowers on the Occasion of his 70th Birthday!

9:00 - 12:00 PARTY

Sunday, January 18

8:00 – 9:00 BREAKFAST

SESSION IV Presider: Hao Chen

9:00 – 9:25 “Structural Studies of Small Peptide Oligomers Using Ion Mobility Mass Spectrometry”, **Christian Bleiholder**, Nick Dupuis, Michael T. Bowers*”, *University of California, Santa Barbara, CA.*

9:25 - 9:50 “Pulsed Q Dynamic Collision Induced Dissociation, a New Approach for Fast Fragmentation in the Quadrupole Ion Trap”, **Unige A. Laskay**, Shannon L. Cook, and Glen P. Jackson*, *University of Arizona, Tucson, AZ.*

9:50 – 10:15 “Increasing Charge While Preserving Noncovalent Protein Complexes for ESI-MS”, **Shirley H. Lomeli**, Sheng Yin, Rachel R. Ogorzalek Loo, and Joseph A. Loo*, *University of California, Los Angeles, CA.*

10:15 – 10:35 BREAK

10:35 – 11:00 “Radical Exchange Between Noncovalently Complexed Peptide Ions”, **Geoffrey K. Yeh**, Jolene K. Deidrich, Tony Ly, Claudia Meneses, and Ryan R. Julian*, *University of California, Riverside, CA.*

11:00 – 11:25 “Differentiating Diastereomeric Peptides by Mass Spectrometry”, **Aaron Moehlig** and Thomas H. Morton*, *University of California, Riverside, CA.*

11:25 - 11:50 “Applications of Large Peptide Clusters”, **Tawnya Flick**, William A. Donald, Ryan Leib, and Evan R. Williams*, *University of California, Berkeley, CA.*

11:50 - 12:00 CHECK OUT

12:00 - 1:00 LUNCH AND DEPART

List of Participants at the 2009 Conference on Ion Chemistry and Mass Spectrometry January 16–18, 2009 UCLA Conference Center, Lake Arrowhead, California

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