

Ion Activation: Fundamentals, Applications and New Frontiers

Organized by

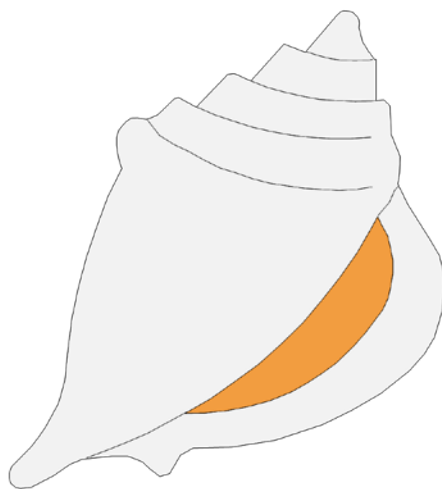
Ryan Julian

UC Riverside

&

Richard Vachet

U. Massachusetts Amherst



26th ASMS Sanibel Conference on Mass Spectrometry
January 30 - February 2, 2014
Clearwater Beach, FL

Erin Baker
PNNL

Sanibel Conference Committee
Neil Kelleher
Northwestern University

JC Poutsma
College of William & Mary

Jon D. Williams
GlaxoSmithKline

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Ryan Julian
UC Riverside



Richard Vachet
U. Massachusetts Amherst

Speakers – please arrive ½ hour before your session to load your presentation.

THURSDAY, JANUARY 30

6:00 – 7:00 pm **Registration, Outside Ballroom F&G**

7:00 – 8:00 pm

Opening Session

Ion Activation: Fundamentals, Applications and New Frontiers

Session Chairs, Richard Vachet, *U. Massachusetts Amherst*

& Ryan Julian, *UC Riverside*

Ballroom F&G

7:00 – 8:00 pm **Evan Williams, UC Berkeley, "How Hot are Your Ions? –
Thermochemistry with Photon, Electron and Collisional Activation"**

8:00 – 10:00 pm

Reception

setup all posters

Water's Edge Ballroom

FRIDAY, JANUARY 31

7:00 - 8:30 am
Continental Breakfast
Water's Edge Ballroom

8:30 – 11:30 am
Photon Based Activation
Session Chair: Gavin Reid, *Michigan State University*
Ballroom F&G

- 8:30 – 8:55 am **Jim Reilly**, *Indiana University*, “Peptides from Antibodies and Libraries: What can we learn from their Photofragmentation?”
- 8:55 – 9:00 am Questions
- 9:00 – 9:25 am **Stephen Blanksby**, *University of Wollongong*, “Alternative Approaches to Ion Activation for Structure Elucidation in Lipidomics”
- 9:25 – 9:30 am Questions
- 9:30 – 9:55 am **Nick Polfer**, *University of Florida*, “Phosphate Scrambling revealed by Infrared Spectroscopy”
- 9:55 – 10:00 am Questions
- 10:00 – 10:30 am **Coffee Break**, *Water's Edge Ballroom*
- 10:30 – 10:55 am **Gary Glish**, *UNC Chapel Hill*, “Ion Excitation/Dissociation in Quadrupole Ion Traps using IR Photons: Are all Slow Heating Methods the Same?”
- 10:55 – 11:00 am Questions
- 11:00 – 11:25 am **Philippe Dugourd**, *University of Lyon*, “Laser Activation of Multiply-charged Biomolecules: from Proteins to Megadalton DNA”
- 11:25 – 11:30 am Questions
- 11:30am – 1:00 pm **Group Lunch**, *Sandpiper Blue Heron Deck*

FRIDAY, JANUARY 31

1:00 – 3:00 pm

Activation of Really BIG Ions

Session Chair: Jennifer Brodbelt

Ballroom F&G

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|----------------|--|
| 1:00 – 1:25 pm | Michal Sharon , <i>Weizmann Institute of Science</i> , “Breaking apart Protein Complexes for Structure/Function Determination” |
| 1:25 – 1:30 pm | Questions |
| 1:30 – 1:55 pm | Vicki Wysocki , <i>Ohio State University</i> , “Coupling Surface–Induced Dissociation and Ion Mobility to Determine Structures of Nucleoproteins and Other Complexes” |
| 1:55 – 2:00 pm | Questions |
| 2:00 – 2:25 pm | Brandon Ruotolo , <i>University of Michigan</i> , "Collision Induced Unfolding of Multiprotein–Ligand Complexes" |
| 2:25 – 2:30 pm | Questions |
| 2:30 – 2:55 pm | Yury Tsybin , <i>Ecole Polytechnique Federale de Lausanne</i> , "Antibodies Structure Analysis by Top–Down and Middle–Down Mass Spectrometry" |
| 2:55 – 3:00 pm | Questions |
| 3:00 – 7:00 pm | Free Time |

7:00 pm – 8:00 pm

Harnessing Odd Activation & Promoted Talks

Session Chair: Kicki Hakansson, *University of Michigan*

Ballroom F&G

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|----------------|--|
| 7:00 – 7:25 pm | Ryan Julian , <i>UC Riverside</i> , “Leveraging Dissociation for more than just Structure or Sequence” |
| 7:25 – 7:30 pm | Questions |
| 7:30 – 7:40 pm | Poster # 15: Xiaoxiao Ma , <i>Purdue University</i> , "Paternò–Büchi Reaction coupled with Mass Spectrometry Allows Facile and Accurate Localization of Double Bonds" |
| 7:40 - 7:45 pm | Questions |
| 7:45 - 7:55 pm | Poster # 25: Christopher Shaffer , <i>University of Washington</i> , " UV Photoreactivity in a Modified Ion Trap" |
| 7:55 - 8:00 pm | Questions |

8:00 – 10:00 pm

Poster Session I

odd–numbered posters present

Water's Edge Ballroom

SATURDAY, FEBRUARY 1

7:00 - 8:30 am
Continental Breakfast
Water's Edge Ballroom

8:30 – 11:30 am
Electron Based Activation
Session Chair: Jack Beauchamp, *Caltech*
Ballroom F&G

- 8:30 – 8:55 am **Helen Cooper**, *University of Birmingham*, “Ion Mobility Mass Spectrometry and Electron Mediated Dissociation for interrogating the Conformational Preferences of Phosphopeptides”
- 8:55 – 9:00 am Questions
- 9:00 – 9:25 am **Frank Turecek**, *University of Washington*, “Structures and Electronic States of Tightly Folded Peptide Cation–Radicals”
- 9:25 – 9:30 am Questions
- 9:30 – 9:55 am **Richard Vachet**, *U. Massachusetts Amherst*, “Characterizing Salt Bridges in Gas–Phase Protein Ions using ETD and CID”
- 9:55 – 10:00 am Questions
- 10:00 – 10:30 am **Coffee Break**, *Water's Edge Ballroom*
- 10:30 – 10:55 am **Michael Gross**, *Washington University*, “ECD and Ion Mobility for Large Proteins and Protein Complexes”
- 10:55 – 11:00 am Questions
- 11:00 – 11:25 am **Jonathan Amster**, *University of Georgia*, “Electron Based Methods of Activation for MS/MS of Anionic Carbohydrates”
- 11:25 – 11:30 am Questions
- 11:30am – 1:00 pm **Lunch**, *on your own*

SATURDAY, FEBRUARY 1

1:00 pm – 3:00 pm

Applications of Site-selective Dissociation

Session Chair: Ryan Julian, *UC Riverside*

Ballroom F&G

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|----------------|---|
| 1:00 – 1:25 pm | Gavin Reid , <i>Michigan State University</i> , “Derivatization Strategies for Multiplexed Lipid Quantification” |
| 1:25 – 1:30 pm | Questions |
| 1:30 – 1:55 pm | Catherine Costello , <i>Boston University</i> , “Developing MS-Based Strategies to Fully Elucidate Glycan Structures” |
| 1:55 – 2:00 pm | Questions |
| 2:00 – 2:25 pm | Jack Beauchamp , <i>Caltech</i> , “Raise the Energy or Lower the Barrier? for Biopolymer Structure Determination the Latter has Unique Advantages” |
| 2:25 – 2:30 pm | Questions |
| 2:30 – 2:55 pm | Jennifer Brodbelt , <i>University of Texas, Austin</i> , “Exploiting Chromophore-Selectivity for UV Photodissociation of Biomolecules” |
| 2:55 – 3:00 pm | Questions |
| 3:00 – 7:00 pm | Afternoon Free |

7:00 – 8:00 pm

Electron based Activation & Promoted Talks

Session Chair: Glen Jackson, *West Virginia University*

Ballroom F&G

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|----------------|---|
| 7:00 – 7:25 pm | Kristina Hakansson , <i>University of Michigan</i> , “Fundamentals and Applications of Gas-Phase Anion-Electron Reactions” |
| 7:25 – 7:30 pm | Questions |
| 7:30 – 7:40 pm | Poster # 4: Russell Bornschein , <i>University of Michigan</i> , “Ion Mobility-Mass Spectrometry Reveals Previously-Unknown Intermediate Forms in the Collision Induced Dissociation of Protein Complexes” |
| 7:40 - 7:45 pm | Questions |
| 7:45 - 7:55 pm | Poster # 16: Lindsay Morrison , <i>Ohio State University</i> , “The Stability of Helical b Ions from XA12K2+ Peptides” |
| 7:55 - 8:00 pm | Questions |

8:00 – 10:00 pm

Poster Session II

even-numbered posters present

Water's Edge Ballroom

SUNDAY, FEBRUARY 2

7:00 - 8:30 am
Continental Breakfast
Water's Edge Ballroom

8:30 – 10:00 am
Molecular Fender-Benders
Session Chair: Helen Cooper, *University of Birmingham*
Ballroom F&G

- 8:30 – 8:55 am **Julia Laskin**, *PNNL*, “Activation and Dissociation of Non-covalent Complexes Using Ion–Surface Collisions”
- 8:55 – 9:00 am Questions
- 9:00 – 9:25 am **Dave Russell**, *Texas A&M*, “Development of Ion Mobility–Mass Spectrometry Approaches as Top–Down Structural Probes”
- 9:25 – 9:30 am Questions
- 9:30 – 9:55 am **Peter Armentrout**, *University of Utah*, “Energetics from Collision induced Dissociation”
- 9:55 – 10:00 am Questions
- 10:00 – 10:30 am **Coffee Break**, *Water's Edge Ballroom*

10:30 - 11:30 am
New Directions
Session Chairs, Richard Vachet
Ballroom F&G

- 10:30 – 10:55 am **Yu Xia**, *Purdue University*, “Reactions of Carbon Centered Radicals with Biomolecule Ions”
- 10:55 – 11:00 am Questions
- 11:00 – 11:25 am **Glen Jackson**, *West Virginia University*, “Metastable Atom activated Dissociation (MAD); Status and Outlook”
- 11:25 am – 11:30 am Questions
- 11:30 – 11:35 am **Closing Remarks**

Poster List

All posters are located in the Water's Edge Ballroom

All posters should be set up by 7:00 pm on Thursday

Remove all posters by 10:30 am on Sunday

odd-numbered posters will be presented on Friday from 8:00 - 10:00 pm

even-numbered posters will be presented on Saturday from 8:00 - 10:00 pm

- 1 **Measurement of the Effect of Yumberry on the Bioavailability of Ranitidine in Rabbits Utilizing the Complementary Utility of UPLC-QQQ and UPLC-QTOF**, Mohamed F. AlAjmi, *College of Pharmacy, King Saud University, Riyadh, Saudi Arabia*
- 2 **Ion-Molecule Reactions and Separation of $^{238}\text{U}/^{238}\text{Pu}$ Isobars in the Collision/Reaction Cell of a Tandem Inductively Coupled Plasma Mass Spectrometer**, Saeed. H. Al-Meer, Mohamed A. Amr, Muneera T. Al-Qahtani, *Central Laboratories Unit, Qatar University, Doha, Qatar*
- 3 **Application of an RF "Ion Tunnel" based on Printed Circuit Technology for Ion Transfer and Ion Temperature Manipulation Purposes**, Sonja Klee, Albrecht Brockhaus, Walter Wißdorf, Thorsten Benter, *Institute for Pure and Applied Mass Spectrometry, University of Wuppertal, Wuppertal, Germany*
- 4 **Ion Mobility-Mass Spectrometry Reveals Previously-Unknown Intermediate Forms in the Collision Induced Dissociation of Protein Complexes**, Russell E. Bornschein, Shuai Niu, and Brandon T. Ruotolo, *University of Michigan, Ann Arbor, MI*
- 5 **Novel Ion Mobility-Mass Spectrometry Instrument to Analyze the Dissociation of Protein Complexes**, Rebecca S. Glaskin,¹ Qi Wang,¹ Ruwan Kurulugama,² Alex Mordehai,² and Catherine E. Costello¹, ¹*Boston University School of Medicine, Boston, MA* ²*Agilent Technologies, Santa Clara, CA*
- 6 **Fragmentation of Organic Ions induced by Laser Radiation in a FT-ICR Mass Spectrometer: Influence of the Laser Wavelength and the Pulse Duration**, Claus Gernert, Martin Clemen, Jürgen Grotemeyer, *Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 1, 24118 Kiel, Germany*
- 7 **Conformational Evolution of Peptides following the opening of Disulfide Bridges using Ion Mobility Coupled with Mass Spectrometry**, Hanozin E.¹, Morsa D.¹, De Pauw E.¹ ¹*Chemistry Department, Mass Spectrometry Laboratory, University of Liege, Liege, Belgium*
- 8 **Mechanisms for the Loss of NO_3 from NO_2** , Kameron A. Duncan and Yassin A. Jeilani, *Spelman College, Atlanta, GA*
- 9 **Structural Effects in Electron Capture Dissociation of High-Valence Metal-Peptide Complexes**, Tao Jiang and Kristina Håkansson, *Department of Chemistry, University of Michigan, Ann Arbor, MI*
- 10 **Molecular Dynamics Simulations for Probing Strong Non-Covalent Bond Interactions in Model Phosphopeptides**, Doyong Kim and David H. Russell, *Department of Chemistry, Texas A&M University, College Station, TX*, Helen J. Cooper, *School of Biosciences, University of Birmingham, UK*

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- 11 **Internal Energy of Ions in Desorption Nanoelectrospray**, Karel Lemr¹, Lucie Hartmanová¹, Petr Fryčák¹, František Tureček², Miroslav Sural³, Vladimír Havlíček^{1,1} *RCPTM, Dept. Anal. Chem., Palacký University, 17.listopadu 12, 771 46 Olomouc, Czech Republic, ²Department of Chemistry, University of Washington, Seattle, WA, USA, ³Dept. Organic Chem., Institute of Molecular and Translational Medicine, Palacký University, 17.listopadu 12, 771 46 Olomouc, Czech Republic*
- 12 **Mechanistic Study on Electron Capture Dissociation of the Oligosaccharide-Mg²⁺ Complex**, Yiqun Huang,^{1,2} Yi Pu,^{1,3} Xiang Yu,^{1,2} Catherine E. Costello,^{1,2,3} Cheng Lin^{1,2}. *1. Mass Spectrometry Resource, 2. Department of Biochemistry, Boston University School of Medicine, Boston, MA, 3. Department of Chemistry, Boston University, Boston, MA*
- 13 **Instrumentation and Studies for Gas-phase Ion/Radical Reactions**, Ziqing Lin¹; Lei Tan²; Yu Xia²; Zheng Ouyang^{1,1} *Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; ²Department of Chemistry, Purdue University, West Lafayette, IN*
- 14 **Atmospheric Pressure Thermal Dissociation-Post-Electrospray Ionization Mass Spectrometry of Biomolecules**, Pengyuan Liu, Hao Chen*, *Center for Intelligent Chemical Instrumentation, Department of Chemistry and Biochemistry, Clippinger Laboratories, Ohio University, Athens, OH*
- 15 **Paternò-Büchi Reaction Coupled with Mass Spectrometry allows Facile and Accurate Localization of Double Bonds**, Xiaoxiao Ma and Yu Xia*, *Department of Chemistry, Purdue University, West Lafayette, IN*
- 16 **The Stability of Helical b Ions from XA₁₂K²⁺ Peptides**, Lindsay J. Morrison and Vicki Wysocki, *Ohio State University, Columbus, OH*
- 17 **Combined use of Ion Mobility and Collision-Induced Dissociation (CID) to investigate the Reactivity of Disulfide-Bridged Peptides in Electron Transfer Dissociation (ETD)**, P.Massonnet^a, G.Upert^b, A.Pastor^b, N.Smargiasso^a, N.Gilles^b, L.Quinton^a and E. De Pauw^a
^aMass Spectrometry Laboratory University of Liège, Belgium, ^bCEA/DSV/iBiTec-S/SIMOPRO, Gif sur Yvette, France
- 18 **The KIT Method: A Kinetic Ion Thermometer for Multiply-Protonated Peptide Ions in the Gas Phase**, Robert Pepin, František Tureček, *Department of Chemistry, University of Washington*
- 19 **Separation and Identification of Isomeric Glycans by Selected Accumulation Ion Mobility Spectrometry and Electron Activated Dissociation**, Yi Pu¹, Mark E. Ridgeway², Melvin A. Park², Cheng Lin³, Catherine E. Costello^{1,3,1} *Department of Chemistry, Boston University, Boston, MA; ²Bruker Daltonics, Billerica, MA; ³Department of Biochemistry, Boston University School of Medicine, Boston, MA*
- 20 **Activation Energy and Oscillator RRKM Relationships: Carbohydrate Structural Details**, Vern Reinhold and Hailong Zhang, *Glycomics Center, University of New Hampshire, Durham, NH*

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- 21 **Base-Pairing Energies of Proton-Bound Dimers of Cytosine and Modified Cytosines: Implications for the Effects of Methylation and Halogenation on the Stability of DNA i-Motif Conformations**, Bo Yang,¹ Aaron. R. Moehlig,² Thomas. H. Morton,² M. T. Rodgers^{1,*},
¹Department of Chemistry, Wayne State University, Detroit, MI, ²Department of Chemistry, University of California, Riverside, CA
- 22 **Verification of Peptic Fragments from Human Insulin Bound Congo Red by ECD: An Application in Pulsed labeling Hydrogen-Deuterium Exchange Coupled with Mass Spectrometry**, Teerapat Rojsajakul, Fred L. King, Department of Chemistry, West Virginia University, Morgantown, WV
- 23 **Use of Top Down ETD based Mass Spectrometry approaches for the High Throughput Clinical Diagnosis of Hemoglobinopathies**, James Scrivens¹; Baharak Vafadar-Isfahani¹; Julia Smith²; Jane Newbold³; Nicholas Jackson³; Krisztina Radi¹, ¹ University of Warwick, School of Life Sciences, Coventry; ² Bruker UK Limited, Coventry; ³ University Hospitals Coventry and Warwickshire, Coventry
- 24 **Affect of Pyrolysis Temperature on CID/MS/MS Spectra**, Sandra E. Spencer, Gary L. Glish, University of North Carolina, Chapel Hill, NC
- 25 **UV Photoreactivity in a Modified Ion Trap**, Christopher J. Shaffer, Robert Pepin, Aleš Marek, and František Tureček*, University of Washington*, Seattle, WA