

## Table of Contents

Program Schedule .....	1
Poster List .....	7
Abstracts .....	15
Directory of Participants .....	79
Blank pages for notes .....	86



**Carol Robinson** obtained her PhD in mass spectrometry from the University of Cambridge. She is currently a Royal Society Research Professor at the University of Oxford. Her research interests include all aspects of mass spectrometry applied to the elucidation of the 3D architecture and structure of macromolecular complexes. Recent highlights from her work include the discovery that membrane protein complexes can be liberated from micelles in the gas phase while retaining their subunits interactions, lipid binding properties and overall topology.



**Brian T. Chait** is currently Camille and Henry Dreyfus Professor at Rockefeller University in New York, where he is Head of the Laboratory for Mass Spectrometry and Gaseous Ion Chemistry. He also directs the NIH-funded National Resource for the Mass Spectrometric Analysis of Biological Macromolecules. Dr. Chait's laboratory specializes in the development and use of mass spectrometry as a tool for investigating a variety of biological and biochemical phenomena. He has co-authored some 334 publications (cited >33,000 times) and has been awarded 23 US patents.

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

## THURSDAY, JANUARY 19

6:00 – 7:00 pm      **Registration**, *Outside of the Tarpon/Sawyer Ballroom*

<b>7:00 – 8:00 pm</b> <b>Opening Session</b> Session Chair, Brandon T. Ruotolo, <i>University of Michigan</i> <i>Tarpon/Sawyer Ballroom</i>
--

7:00 - 7:10 pm	<b>Opening Remarks</b>
7:10 – 8:10 pm	<b>Opening Lecture: Carol Robinson</b> , <i>University of Oxford</i> Mass Spectrometry and its Role in Structural Biology

<b>8:00 - 10:00 pm</b> <b>Reception</b> setup all posters <i>Banyan Breezeway</i>
--

## FRIDAY, JANUARY 20

<b>8:30 – 11:20 am</b> <b>Structural Characterization by Ion Mobility</b> Session Chair: Matt Bush, <i>University of Washington</i> <i>Tarpon/Sawyer Ballroom</i>
--

8:30 – 9:00 am	<b>David Clemmer</b> , <i>Indiana University</i> Conformations of Peptides and Proteins Emerging from Solution into the Gas Phase
9:00 – 9:30 am	<b>Julie Leary</b> , <i>UC Davis</i> Protein-Carbohydrate Interactions: Ion Mobility and RAPTOR Analysis for Isomeric Differentiation
9:30 - 9:50 am	<b>Coffee Break</b> , <i>Banyan Breezeway</i>
9:50 – 10:20 am	<b>Joseph Loo</b> , <i>UCLA</i> Utility of Mass Spectrometry/Ion Mobility for Defining Protein-Ligand and Protein-Protein Interactions Important in Biology and Medicine
10:20 – 10:50 am	<b>Albert Heck</b> , <i>Utrecht University</i> Structural Characterization of Virus Assembly using Native Ion Mobility Mass Spectrometry
10:50 – 11:20 am	<b>Brandon T. Ruotolo</b> , <i>University of Michigan</i> Collision Induced Unfolding (CIU) Applied to Frontier Challenges in Structural Biology and Protein-Ligand Binding
11:20 – 11:40 am	<b>Coffee Break</b> , <i>Banyan Breezeway</i>

**FRIDAY, JANUARY 20**

**11:40 am - 12:40 pm**

**Structural Characterization by Ion Activation/Fragmentation I**

Session Chair: Frank Sobott, *University of Antwerp*

*Tarpon/Sawyer Ballroom*

- 11:40 am - 12:10 pm **Justin Benesch**, *University of Oxford*  
Determining the Likely Structures of Polydisperse Proteins
- 12:10 - 12:40 pm **Vicki Wysocki**, *University of Arizona*  
SID/IM and IM/SID: Useful Approaches for Characterization of Non-Covalent Complexes
- 12:40 – 2:00 pm **Group Lunch**, *Garden Courtyard*

**2:00 - 3:30 pm**

**Structural Characterization by Ion Activation/Fragmentation II**

Session Chair: Frank Sobott, *University of Antwerp*

*Tarpon/Sawyer Ballroom*

- 2:00 - 2:30 pm **John Klassen**, *University of Alberta*  
Structure and Stability of Protein-Ligand Complexes in the Gas Phase
- 2:30 - 3:00 pm **Nick Polfer**, *University of Florida*  
Unscrambling the CID Fragmentation Chemistry of Peptides
- 3:00 - 3:30 pm **Evan Williams**, *UC Berkeley*  
Supercharging Proteins from Native Solutions: Mechanisms and Applications

**7:00 - 8:00 pm**

**Promoted Talks I**

Session Chair: Justin Benesch, *University of Oxford*

*Tarpon/Sawyer Ballroom*

- 7:00 - 7:15 pm **Frank Sobott**, *University of Antwerp*  
*Poster 7* - What do Ion Mobility Measurements tell us about the Conformational Space of Proteins and Protein Complexes?
- 7:15 - 7:30 pm **A. E. Ashcroft**, *University of Leeds*  
*Poster 9* - Exploring Lactococcal Phage Baseplate Assembly
- 7:30 - 7:45 pm **Esther van Duijn**, *Utrecht University*  
*Poster 18* - Structural Characterization of CRISPR-Associated Immunity Complexes
- 7:45 - 8:00 pm **Owen Nadeau**, *University of Kansas Medical Center*  
*Poster 26* - Mass Spectrometry Reveals Different Subunit Interaction Maps for the Native and Phosphorylated Conformers of the (abgd)<sub>4</sub> Phosphorylase Kinase Complex

**8:00 - 10:00 pm**

**Poster Session I**

posters 1 - 29

*Banyan Breezeway*

**SATURDAY, JANUARY 21**

**8:30 - 10:30 am**

**Structural Characterization by Hydrogen/Deuterium Exchange**

Session Chair: Thomas Wales, *Northeastern University*

*Tarpon/Sawyer Ballroom*

- 8:30 - 9:00 am **John Engen**, *Northeastern University*  
Protein Flexibility and Plasticity
- 9:00 - 9:30 am **Michael Fitzgerald**, *Duke University*  
Covalent Labeling Strategy for the Large Scale and High-Throughput  
Analysis of Protein-Ligand Binding
- 9:30 - 10:00 am **Igor Kaltashov**, *University of Massachusetts*  
Protein Dynamics and Interactions: Using Ion-Electron Interactions to  
Enhance Quality and Resolution of Native ESI MS and HDX MS  
Measurements
- 10:00 - 10:30 am **Alan Marshall**, *NHMFL/Florida State University*  
H/D Exchange for Mapping Contact Surfaces in Large Protein  
Complexes
- 10:30 - 11:00 am **Coffee Break**, *Banyan Breezeway*

**11:00 am - 12:30 pm**

**Labeling Strategies for Structural Characterization**

Session Chair: Nick Polfer, *The University of Florida*

*Tarpon/Sawyer Ballroom*

- 11:00 - 11:30 am **Lars Konermann**, *University of Western Ontario*  
Oxidative Labeling and HDX-MS As Complementary Tools for Probing  
Membrane Protein Structure and Function
- 11:30 - 12:00 **Mark Chance**, *Case Western Reserve University*  
Structural Mass Spectrometry: Dynamics of Membrane Proteins
- 12:00 - 12:30 pm **Ryan Julian**, *UC Riverside*  
Examination of Surface Structure in Highly Homologous Proteins with  
SNAPP-MS
- 12:30 - 12:45 pm **Alexander Leitner**, *ETH Zurich*  
*Poster 47* - Probing the Topology of Large Protein Complexes Using  
Chemical Cross-Linking and Mass Spectrometry
- 12:45 - 1:00 pm **Gavin Reid**, *Michigan State University*  
*Poster 52* - Oxidation Induced Conformational Changes in Calcineurin  
Studied by 'Fixed Charge' Chemical Derivatization and Data Dependent  
Multistage Tandem Mass Spectrometry
- 1:00 - 7:00 pm **Afternoon Free**

**SATURDAY, JANUARY 21**

**7:00 - 8:00 pm**

**Promoted Talks II**

Session Chair: Natalia Carulla, *Institut de Recerca Biomèdica (IRB)*

*Horizons Ballroom*

- 7:00 - 7:15 pm **Kerry M. Hassell**, *Northeastern University*  
*Poster 37 - Solution-Phase Hydrogen Exchange Followed by Electron Transfer Dissociation for Analysis of Conformational Features of Proteins*
- 7:15 - 7:30 pm **Matthias P. Mayer**, *Zentrum für Molekulare Biologie der Universität Heidelberg (ZMBH)*  
*Poster 43 - Conformational Dynamics of Hsp90 Chaperones Analyzed by Hydrogen Exchange Mass Spectrometry*
- 7:30 - 7:45 pm **Romina Hofele**, *Max Planck Institute for Biophysical Chemistry*  
*Poster 51 - DEAH Box Helicase Prp43-Ntr1 Complex: Insights into Structure Combining Oxidative Footprinting with Protein-RNA Cross-Linking and Mass Spectrometry*
- 7:45 - 8:00 pm **John O'Brien**, *University of Texas at Austin*  
*Poster 57 - Evaluating Protein Solvent Accessibility via Electron Transfer Dissociation and 351 nm Ultraviolet Photodissociation Mass Spectrometry*

**8:00 - 10:00 pm**

**Poster Session II**

posters 30 - 65

*Banyan Breezeway*

*remove all posters by 10:30 pm*

**SUNDAY, JANUARY 22**

**9:00 - 10:00 am**

**Emerging Directions and Techniques**

Session Chair: Esther van DuJin, *Utrecht University*

*Tarpon/Sawyer Ballroom*

- 9:00 - 9:30 am **David Russell**, *Texas A&M University*  
Enhanced Sampling MDS and IM-MS Studies of Environment-Dependent Conformer Preferences of Amphipathic Membrane-Active Peptides
- 9:30 - 10:00 am **Scott McLuckey**, *Purdue University*  
Ion/Ion Reactions for Protein Cross-linking of Gaseous Polypeptide Ions
- 10:00 - 10:15 am **Coffee Break**, *Lobby*
- 10:15 - 10:45 am **Richard Smith**, *Pacific Northwest National Laboratory*  
Advances in Applications of Separations with Mass Spectrometry for the Broad Characterization of Complex Biological Systems
- 10:45 - 11:15 am **John A. McLean**, *Vanderbilt University*  
Structurally-Based Discovery Strategies for Complex Biological Systems
- 11:15 - 11:30 am **Coffee Break**, *Lobby*

**11:30 am - 12:45 pm**

**Closing Session**

Session Chair, John A. McLean, *Vanderbilt University*

*Tarpon/Sawyer Ballroom*

- 11:30 - 12:30 pm **Closing Lecture: Brian Chait**, *Rockefeller University*  
On the Role of Mass Spectrometry in Structural Biology: The Present and Future
- 12:30 - 12:45 pm **Closing Remarks**

## Poster List

All posters are located in the Banyan Breezeway  
posters 1 - 29 will be presented on Friday from 8:00 - 10:00 pm  
posters 30 - 65 will be presented on Saturday from 8:00 - 10:00 pm  
All posters should be set up by 7:00 pm on Thursday  
Remove all posters by 10:30 pm on Saturday

### Poster Topic

#### Structural Characterization by Ion Mobility

- 1 **Trapped Ion Mobility Spectrometry (TIMS) as a Tool for Gas Phase Ion Structure Studies;** Mark E. Ridgeway<sup>1</sup>, Desmond Kaplan<sup>1</sup>, Goekhan Baykut<sup>2</sup>, Melvin Park<sup>1</sup>; <sup>1</sup> Bruker Daltonics, 40 Manning Road, Billerica, MA and <sup>2</sup> Bruker Daltonik GmbH, Bremen, Germany
- 2 **Study of Oligomeric Forms of the Alzheimer's Disease-Related Amyloid- $\beta$  (A $\beta$ ) Protein;** Rosa Pujol-Pina,<sup>1</sup> Ernest Giralt,<sup>1,2</sup> Natàlia Carulla<sup>1</sup>; <sup>1</sup>Institute for Research in Biomedicine (IRB Barcelona), Barcelona, Spain. and <sup>2</sup>Department of Organic Chemistry, University of Barcelona, Barcelona, Spain.
- 3 **Conformational Dynamics Study of Prolyl Oligopeptidase by Ion Mobility Mass Spectrometry;** Abraham López<sup>1,2</sup>, Teresa Tarragó<sup>1</sup>, Marta Vilaseca<sup>3</sup>, Sergio Madurga<sup>4</sup>, Ernest Giralt<sup>1,2</sup>; <sup>1</sup> Institute for Research in Biomedicine (IRB-Barcelona). Baldiri Reixach, 10, 08028, Barcelon, <sup>2</sup> Department of Organic Chemistry, University of Barcelona (UB), <sup>3</sup> Mass Spectrometry Core Facility, IRB-Barcelona, <sup>4</sup> Department of Physical Chemistry, University of Barcelona (UB).
- 4 **Characterization of Structural Changes of Metallothionein by Ion Mobility-Mass Spectrometry (IM-MS): Metal-Free vs. Metallated Forms;** Shu-Hua Chen and David H. Russell; Department of Chemistry, Texas A&M University, College Station, TX
- 5 **A Simple Damping Factor Links Periodic Focusing and Uniform Field Ion Mobility Measurements for Accurate Determination of Collision Cross Sections;** Joshua A. Silveira, Chaminda M. Gamage, Junho Jeon, Pei-Jing Pai, Kyle L. Fort, David H. Russell; Texas A&M University, Department of Chemistry, Laboratory for Biological Mass Spectrometry, College Station, TX
- 6 **Protein Interactions with Synthetic Polymers: Do Structural Changes Occur?;** Vincenzo Scionti and Chrys Wesdemiotis; The University of Akron, Department of Chemistry, Akron, OH
- 7 Promoted poster 15-minute talk during the Friday Promoted Talks I session - **What do Ion Mobility Measurements tell us about the Conformational Space of Proteins and Protein Complexes?;** Frank Sobott; University of Antwerp, CFP-CeProMa and Chem. Dept., Antwerp, Belgium
- 8 **Ion Mobility Mass Spectrometry of DNA/SgrAI Nuclease Oligomers;** Xin Ma, Mowei Zhou, Chad K. Park, Santosh Shan, Vicki H. Wysocki and Nancy C. Horton; Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ
- 9 Promoted poster 15-minute talk during the Friday Promoted Talks I session - **Exploring Lactococcal Phage Baseplate Assembly;** D. A. Shepherd<sup>1</sup>, D. Veessler<sup>2</sup>, J. Lichière<sup>2</sup>, C. Cambillau<sup>2</sup>, A. E. Ashcroft<sup>1\*</sup>; <sup>1</sup> Astbury Centre for Structural Molecular Biology & Faculty of Biological Sciences, University of Leeds, Leeds, UK and <sup>2</sup> Architecture et Fonction des Macromolécules Biologiques, UMR 6098 CNRS & Universités Aix-Marseille I & II, Marseille, France

*Poster Topic*  
**Structural Characterization by Ion Mobility**

- 10 **A Tale of a Tail: Structural Insights into Ataxin-3 Gained by Ion Mobility Spectrometry - Mass Spectrometry;** Charlotte A. Scarff, Alessandro Sicorello, Sheena E. Radford, Alison E. Ashcroft; *The Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK*
- 11 **A Conformational Study of the Hepatitis B Core Antigen by Non-Covalent Mass Spectrometry and Ion Mobility Spectrometry- Mass Spectrometry;** Dale A. Shepherd, Kris K. Holmes, Nicola J. Stonehouse, Alison E. Ashcroft; *The Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK*
- 12 **Gas-phase Multiprotein Complexes: Preserving Native-like Structures via Optimized Buffer Conditions;** Linjie Han, Suk-Joon Hyung, and Brandon T. Ruotolo; *Department of Chemistry, University of Michigan, Ann Arbor*
- 13 **An Integrated Structural Biology Dataset Reveals Metal-Protein and Protein-Protein Interactions of Critical Importance for Amyloid Formation;** Suk-Joon Hyung<sup>1</sup>; Molly Soper<sup>1</sup>; Mi Hee Lim<sup>1,2</sup>; Brandon Ruotolo<sup>1</sup>; *Department of Chemistry<sup>1</sup> and Life Science Institute<sup>2</sup>, University of Michigan, Ann Arbor, MI*
- 14 **Collision Induced Unfolding of Multi-Protein Ligand Complexes: Using Ion Mobility-Mass Spectrometry to Study the Concanavalin A –Sugar Binding System;** Shuai Niu, Suk-Joon Hyung, Brandon T. Ruotolo; *University of Michigan, Ann Arbor, MI*
- 15 **Developing Ion Mobility-Mass Spectrometry as a Novel High Throughput Screening Method for Protein Tyrosine Kinase Inhibitors;** Jessica Rabuck, Sukjoon Hyuang, Brandon Ruotolo; *Department of Chemistry, University of Michigan, Ann Arbor, MI*
- 16 **Ion Mobility-Mass Spectrometry Screening Reveals Neuropeptide Interactions with Amyloid b Peptides and their Oligomers;** Molly Soper<sup>1</sup>, Suk-Joon Hyung<sup>1</sup>, Mi Hee Lim<sup>1,2</sup>, and Brandon T. Ruotolo<sup>1</sup>; *Department of Chemistry<sup>1</sup>, Life Science Institute<sup>2</sup>, University of Michigan*
- 17 **Development of Ion Mobility-Mass Spectrometry as a High-throughput Approach for Structural Proteomics;** Yueyang Zhong, Suk-Joon Hyung and Brandon Ruotolo; *Department of Chemistry, University of Michigan, Ann Arbor, MI*
- 18 *Promoted poster 15-minute talk during the Friday Promoted Talks I session -* **Structural Characterization of CRISPR-Associated Immunity Complexes;** Esther van Duijn<sup>1,2##</sup>, Ioana M. Barbu<sup>1,2#</sup>, Arjan Barendregt<sup>1,2</sup>, Matthijs M. Jore<sup>3</sup>, Blake Wiedenheft<sup>4</sup>, Magnus Lundgren<sup>3,5</sup>, Edze R. Westra<sup>3</sup>, Stan J.J. Brouns<sup>3</sup>, Jennifer A. Doudna<sup>4</sup>, John van der Oost<sup>3</sup> and Albert J.R. Heck<sup>1,2\*</sup>; <sup>1</sup>*Biomolecular Mass Spectrometry and Proteomics Group, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, University of Utrecht, Utrecht, The Netherlands,* <sup>2</sup>*Netherlands Proteomics Centre, Utrecht, The Netherlands,* <sup>3</sup> *Wageningen University, Wageningen, The Netherlands* <sup>4</sup> *Department of Molecular and Cell Biology, University of California, Berkeley, CA* and <sup>5</sup> *Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden*
- 19 **Characterization of Carbohydrates and Carbohydrate Natural Products by LC- Ion Mobility-Mass Spectrometry;** Nichole M. Lareau, Larissa S. Fenn, Cody R. Goodwin, Jody C. May, Brian O. Bachmann and John A. McLean; *Department of Chemistry, Vanderbilt Institute of Chemical Biology and Vanderbilt Institute for Integrative Biosystems Research and Education Vanderbilt University, Nashville TN*

*Poster Topic*  
**Structural Characterization by Ion Mobility**

- 20 **Using Distance Geometry with Ion Mobility-Mass Spectrometry Data to Study the Conformational Space of Natural Products;** Sarah M. Stow,<sup>1,2,3,4</sup> Cody R. Goodwin,<sup>1,2,4</sup> Michal Kliman,<sup>1,2,4</sup> Brian O. Bachmann,<sup>1,2</sup> John A. McLean<sup>1,2,4</sup>; *1. Department of Chemistry at Vanderbilt University, 2. Vanderbilt Institute of Chemical Biology, 3. Center for Structural Biology, 4. Vanderbilt Institute for Integrative Biosystems Research and Education, Vanderbilt University, Nashville, TN*

*Poster Topic*  
**Structural Characterization by Ion Activation/Fragmentation**

- 21 **Characterization of New Fatty Acid from *Maytenus* Speices using Fragmentaion Pattern and Mass Behaviour;** Mohamed F. AlAjm\*, PhD.<sup>1</sup> and Maged Saad Abdel-Kader<sup>2</sup>, <sup>1</sup>*Prince Sultan Prince College for emergency medical services, King Saud University, Riyadh, Saudi Arabi* and <sup>2</sup>*College of Pharmacy, Prince Salman University, Kharj, Saudi Arabia*
- 22 **Density Functional Theoretical Studies of Charge-Remote Fragmentations: Toward the Development of Predictive Reactions Mechanisms for Steroids Mass Spectrometry;** Yassin A. Jeilani<sup>1</sup> and Victor M. Ibeanusi<sup>2</sup>; <sup>1</sup>*Department of Chemistry, Spelman College, Atlanta, GA* and <sup>2</sup>*Environmental Science and Studies Program, Spelman College, Atlanta, GA*
- 23 **Modeling Gas-Phase Anion-Molecule Complexes of 1,3,5-Trinitroperhydro-1,3,5-Triazine (RDX);** Dominique Newallo, Nripendra K Bose, Albert Thompson, Yassin Jeilani; *Spelman College*
- 24 **Effect of Charge State on Gas-phase Dissociation Behavior of Non-Covalent Protein Complexes Examined by Ion Mobility-Mass Spectrometry;** Mowei Zhou, Royston Quintyn, Shai Dagan, Vicki Wysocki; *University of Arizona, Tucson, AZ*
- 25 **IRMPD Spectroscopy of  $b_n$  (n=4-12) Fragment Ions “How Large Can Macrocycles Become?”;** Marcus Tirado,<sup>a</sup> Josipa Grzetic,<sup>b</sup> Jos Oomens,<sup>b</sup> and Nick C. Polfer<sup>a</sup>; <sup>a</sup>*Department of Chemistry, University of Florida, Gainesville, FL* and <sup>b</sup>*FOM Institute “Rijnhuizen”, Nieuwegein, The Netherlands*
- 26 **Promoted poster 15-minute talk during the Friday Promoted Talks I session - Mass Spectrometry Reveals Different Subunit Interaction Maps for the Native and Phosphorylated Conformers of the  $(\alpha\beta\gamma\delta)_4$  Phosphorylase Kinase Complex;** Owen W. Nadeau<sup>1</sup> Laura A. Lane<sup>2,3</sup>, Jessica Sage<sup>1</sup>, Gerald M. Carlson<sup>1</sup> and Carol V. Robinson<sup>4</sup>; <sup>1</sup>*Department of Biochemistry and Molecular Biology, University of Kansas Medical Center, Kansas City, KS, .A.,* <sup>2</sup>*Department of Chemistry, University of Cambridge, Cambridge, U.K.,* <sup>3</sup>*Department of Chemistry, Chemistry Research Laboratory, Oxford, U.K.* and <sup>4</sup>*Department of Chemistry, the Physical and Theoretical Chemistry Laboratory, University of Oxford, Oxford, U.K.*
- 27 **Twenty-Seven Years of Neutral Gas Collisions of Carbohydrate Samples; Where are We Now?;** Vern Reinhold, David Ashline, Andy Hanneman, and Hailong Zhang; *The Glycomics Center, University of New Hampshire, Durham, NH*
- 28 **Comparison of Peptoid Fragmentation under CID and IRMPD Conditions;** Jianhua Ren\*, Kiran Morishetti and Bogdan Bogdanov; *University of the Pacific, Stockton, CA*

*Poster Topic*  
**Structural Characterization by Ion Activation/Fragmentation**

- 29 **Evidence for Hydrogen/Deuterium Scrambling in Electron Capture Dissociation – Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Teerapat Rojsajjakul, Thomas P. Neis, and Fred L. King\*, *C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV*

*Poster Topic*  
**Structural Characterization by Hydrogen/Deuterium Exchange**

- 30 **Structural Evidence for Cooperative Microtubule Stabilization by Taxol and the Endogenous Dynamics Regulator MAP4;** Hui Xiao<sup>§</sup>, Hui Wang<sup>¶</sup>, Xuechun Zhang<sup>¶</sup>, Zongcai Tu<sup>¶</sup>, Chloë Bulinski<sup>‡</sup>, Marina Khrapunovich-Baine<sup>#</sup>, Ruth Hogue Angeletti<sup>€</sup>, Susan Band Horwitz<sup>#</sup>, <sup>§</sup>*Department of Pathology*, <sup>#</sup>*Department of Molecular Pharmacology*, <sup>€</sup>*Laboratory of Macromolecular Analysis and Proteomics, Albert Einstein College of Medicine, Bronx, NY*, <sup>¶</sup>*State Key Laboratory of Food Science & Technology, Nanchang University, China* and <sup>‡</sup>*Department of Biological Sciences, Columbia University, New York, NY*
- 31 **Impact of Site-Specific Oxidation on the Higher-Order Structure of Interferon  $\beta$ -1a;** George M. Bou-Assaf, Marek Kloczewiak, Damian Houde, and Steven A. Berkowitz; *Biogen Idec, Inc., Cambridge, MA*
- 32 **Fragment Antibody Binding to a Highly Conserved Influenza Epitope - an HDX Study;** Joomi Ahn\*, Eveline Sneekes-Vriese<sup>¶</sup>, Otto Diefenbach<sup>¶</sup>, Ying Qing Yu\*, Alex Muck\*, St John Skilton\*, Els C.M. Brinkman van der Linden<sup>¶</sup>, Robert H. Friesen<sup>¶</sup> and Adrian C. Apetri<sup>¶, &</sup>, \**Waters Corporation, Milford, MA*, <sup>¶</sup>*Crucell BV, Archimedesweg 4, Leiden, 2333CN, The Netherlands* and <sup>&</sup>*To whom correspondence should be addressed*
- 33 **Identification of Residues that Mediate the Assembly of COPII Cages by H/D Exchange Coupled with FT-ICR MS;** Qian Zhang<sup>2</sup>, Scott M. Stagg<sup>2,3</sup>, Christopher L. Hendrickson<sup>1,2</sup> and Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>*Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*, <sup>2</sup>*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL* and <sup>3</sup>*Department of Biological Science and Institute of Molecular Biophysics, Florida State University, Tallahassee, FL*
- 34 **High Resolution Hydrogen/Deuterium Exchange Mass Spectrometry Gives Insight to the Mechanism of Action of Hepatitis B Virus Capsid Assembly Effectors;** Navid Movahed<sup>1</sup>, Dewey Brooke<sup>1</sup>, Adam Zlotnick<sup>2</sup>, and Brian Bothner<sup>1</sup>; <sup>1</sup>*Dept. Chem. Biochem., Montana State University, Bozeman, MT*; <sup>2</sup>*Dept. Biochem., Indiana University, Bloomington, IN*
- 35 **Changes in a Monoclonal Antibody upon Dimerization as Revealed by HX MS;** Roxana E. Iacob<sup>1</sup>, Damian Houde<sup>2</sup>, Steven Berkowitz<sup>2</sup> and John R. Engen<sup>1</sup>; <sup>1</sup>*Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA*, <sup>2</sup>*Biogen Idec, Inc., Cambridge, MA*
- 36 **Conformational Locking upon Cooperative Assembly of Notch Transcription Complexes;** Sung Hee Choi<sup>1</sup>, Thomas E. Wales<sup>2</sup>, Stephen C. Blacklow<sup>1,3</sup>, and John R. Engen<sup>2</sup>; <sup>1</sup>*Department of Cancer Biology, Dana-Farber Cancer Institute, Boston, MA*; <sup>2</sup>*Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA*; <sup>3</sup>*Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA*

*Poster Topic*  
**Structural Characterization by Hydrogen/Deuterium Exchange**

- 37 *Promoted poster 15-minute talk during the Saturday Promoted Talks III session -* **Solution-Phase Hydrogen Exchange Followed by Electron Transfer Dissociation for Analysis of Conformational Features of Proteins;** Kerry M. Hassell<sup>1</sup>, William B. Smith<sup>1</sup>, Sean Marcisin<sup>1</sup>, Elaine M. Marzluff<sup>1</sup>, Jeffery M. Brown<sup>2</sup>, Michael Morris<sup>2</sup>, Jay Bradner<sup>3</sup>, John R. Engen<sup>1\*</sup>; <sup>1</sup> *Department of Chemistry and Chemical Biology and The Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA,* <sup>2</sup> *Waters MS Technologies Centre, Micromass UK Ltd., Wythenshawe, Manchester, UK* and <sup>3</sup> *Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA*
- 38 **Structural Insight into the Mechanism of Regulation of *Neisseria meningitidis* NadA Expression by the Small Natural Ligand 4-HPA;** Sébastien Brier<sup>1</sup>, Luca Fagnocchi<sup>1,2</sup>, Danilo Donnarumma<sup>1,2</sup>, Maria Scarselli<sup>1</sup>, Rino Rappuoli<sup>1</sup>, Mikkel Nissum<sup>1</sup>, Isabel Delany<sup>1</sup> and Nathalie Norais<sup>1</sup>; <sup>1</sup> *Novartis Vaccines, Microbial Molecular Biology, Via Fiorentina 1, 53100 Siena, Italy* and <sup>2</sup> *Recipient of a Novartis fellowship from the PhD program in Functional Biology of Molecular and Cellular Systems of the University of Bologna.*
- 39 **Beyond Structure Characterization: Structure Dynamics (Hydrogen Deuterium Exchange) Guided Biocatalyst Improvement;** Ugur Uzuner<sup>1</sup>, Weibing Shi<sup>1</sup>, Quentin Johnson<sup>2</sup>, Hong Guo<sup>2</sup>, Joshua S. Yuan<sup>1</sup> and Susie Y. Dai<sup>3</sup>; <sup>1</sup> *Department of Plant Pathology and Microbiology,* <sup>2</sup> *University of Tennessee Knoxville, TN* and <sup>3</sup> *Oak Ridge National Laboratory, Oak Ridge, TN,* <sup>3</sup> *Office of the Texas State Chemist, Department of Veterinary Pathobiology, Texas A&M University, College Station, TX*
- 40 **Identification of Regions of Rabbit Muscle Pyruvate Kinase Important for Allosteric Regulation by Phenylalanine, Detected by H/D Exchange Mass Spectrometry;** Charulata B. Prasannan, Maria T. Villar, Antonio Artigues, and Aron W. Fenton; <sup>1</sup> *Department of Biochemistry and Molecular Biology, The University of Kansas Medical Center, Kansas City, KS*
- 41 **Evidence for an Allosteric Auto-Inhibitory Phosphorylation Mechanism Regulating the Endosomal Localization of MTMR2 using Hydrogen/Deuterium Exchange Mass Spectrometry;** Christopher A. Bonham and Panayiotis O. Vacratsis; *Dept. of Chemistry and Biochemistry, University of Windsor, Windsor ON, Canada*
- 42 **Use of Ion Mobility and Fragment Ions to Increase Coverage in Hydrogen-Deuterium Exchange;** Martha Stapels, <sup>2</sup>Thomas Wales, <sup>1</sup>Keith Fadgen, <sup>1</sup>Michael Eggertson, and <sup>2</sup>John Engen; *Waters Corporation*<sup>1</sup> and *Northeastern University*<sup>2</sup>
- 43 *Promoted poster 15-minute talk during the Saturday Promoted Talks III session -* **Conformational Dynamics of Hsp90 Chaperones analyzed by Hydrogen Exchange Mass Spectrometry;** Chung-Tien Lee, Christian Graf, Franz-Josef Mayer, Minh Nguyen and Matthias P. Mayer; *Zentrum für Molekulare Biologie der Universität Heidelberg (ZMBH), Heidelberg, Germany*

*Poster Topic*  
**Labeling Strategies for Structural Characterization**

- 44 **Characterization of Proinsulin and Diabetes Mellitus-Associated Insulin Mutants by Hydroxyl-radical Footprinting and Molecular Modeling;** Janna G. Kiselar<sup>1</sup>, Manish Datt<sup>1</sup>, Nelson Phillips<sup>3</sup>, Mark R. Chance<sup>1,2</sup> and Michael A. Weiss<sup>3</sup>; <sup>1</sup>*Center for Proteomics and Bioinformatics*, <sup>2</sup>*Center for Synchrotron Biosciences*, <sup>3</sup>*Department of Biochemistry Case Western Reserve University, Cleveland, OH*
- 45 **A Mass Spectrometry-based Carboxyl Footprinting Enrichment Strategy for Detection of Low Abundant Derivatized Peptides;** Erik J. Soderblom, J. Will Thompson and M. Arthur Moseley; *Proteomics Core Facility, Institute for Genome Science & Policy, Duke Univ School of Medicine, Durham, NC*
- 46 **Protein Fluorescence in the Gas Phase: the Green Fluorescent Protein and Protein-Dye Conjugates for Probing the Structure of Gaseous Protein Ions;** Konstantin Barylyuk, Vladimir Frankevich, Pavel Sagulenko, Robert Steinhoff, and Renato Zenobi; *Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland*
- 47 *Promoted poster 15-minute talk during the Saturday Promoted Talks II session -* **Probing the Topology of Large Protein Complexes using Chemical Cross-Linking and Mass Spectrometry;** Alexander Leitner, Franz Herzog, Thomas Walzthoeni, Ruedi Aebersold; *Institute of Molecular Systems Biology, ETH Zurich, 8093 Zurich, Switzerland*
- 48 **Detection of Non-covalent Interactions of Single Stranded DNA with Escherichia Coli Single-Stranded DNA-Binding Protein by MALDI-MS;** Fan Chen, Stefanie Mädler, Simon Weidmann, Renato Zenobi; *Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich, Switzerland*
- 49 **Concatenated Protein Oligomers for High-Mass MALDI-MS Calibration;** Simon Weidmann, Konstantin Barylyuk, Stefanie Mädler, Renato Zenobi; *Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland*
- 50 **Observing the Binding Site and Dynamics of Protein S1 on a Bacterial Ribosome using Cross-Linking and Mass Spectrometry;** Matthew A. Lauber<sup>1</sup>, Juri Rappsilber<sup>2</sup>, and James P. Reilly<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Indiana University, Bloomington, IN*, <sup>2</sup>*Wellcome Trust Centre for Cell Biology, Institute of Cell Biology, The University of Edinburgh, Edinburgh, UK*
- 51 *Promoted poster 15-minute talk during the Saturday Promoted Talks III session -* **DEAH Box Helicase Prp43-Ntr1 Complex: Insights into Structure Combining Oxidative Footprinting with Protein-RNA Cross-Linking and Mass Spectrometry;** Romina Hofele<sup>1</sup>, Henning Christian<sup>2</sup>, Ralf Ficner<sup>2</sup>, Henning Urlaub<sup>1,3</sup>; <sup>1</sup>*Max Planck Institute for Biophysical Chemistry, Göttingen, Germany*; <sup>2</sup>*Institute for Microbiology and Genetics, Georg August Universität Göttingen, Germany*; <sup>3</sup>*University Medical Center Göttingen*
- 52 *Promoted poster 15-minute talk during the Saturday Promoted Talks II session -* **Oxidation Induced Conformational Changes in Calcineurin Studied by 'Fixed Charge' Chemical Derivatization and Data Dependant Multistage Tandem Mass Spectrometry;** Gavin E. Reid; *Department of Chemistry, Department of Biochemistry, Michigan State University, East Lansing, MI*
- 53 **Studying Structures and Conformation Dynamics of Peptides and Proteins Using Host-Guest Chemistry in the Gas Phase;** Hugh I. Kim; *Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, S. Korea*

*Poster Topic*  
**Labeling Strategies for Structural Characterization**

- 54 **Understanding the Protein-Protein Interactions of the Human Fe-S Cluster Complex using Hydroxyl Radical Footprinting;** Michaella J. Levy, Pei-Jing Pai, David H. Russell, David P. Barondeau; *Texas A&M University*
- 55 **A Computational Data Analysis Platform for Identifying Zero-Length Chemical Crosslinks using Tandem Mass Spectrometry;** Sira Sriswasdi<sup>1,2</sup>, Sandra Harper<sup>1</sup>, Hsin-Yao Tang<sup>1</sup>, and David W. Speicher<sup>1,2</sup>; <sup>1</sup>*The Wistar Institute, Philadelphia, PA*, <sup>2</sup>*Genomics and Computational Biology Graduate Group, University of Pennsylvania, Philadelphia, PA*
- 56 **Xlink-Identifier 2.0: Identifying Modified Cross-linked Peptides using Tandem Mass Spectrometry and Parallel Computing;** Wenchao Zhang,<sup>†</sup> Kyle Suttlemyre,<sup>†</sup> Peter Pham,<sup>†</sup> James Rorie,<sup>†</sup> Xiuxia Du<sup>†\*</sup>,<sup>†</sup> *Department of Bioinformatics & Genomics, University of North Carolina at Charlotte, NC*
- 57 *Promoted poster 15-minute talk during the Saturday Promoted Talks III session -* **Evaluating Protein Solvent Accessibility via Electron Transfer Dissociation and 351 nm Ultraviolet Photodissociation Mass Spectrometry;** John O'Brien, Jennifer Brodbelt; *Department of Chemistry and Biochemistry, University of Texas at Austin*

*Poster Topic*  
**Emerging Directions and Techniques**

- 58 **Does the Whole Influence the Parts in an Fc Fusion Protein?;** Damian Houde and Steven A. Berkowitz; *Biogen Idec, Inc., Cambridge, MA*
- 59 **Strong Metal Ions Bind Peptides in the Iminol Conformation;** Robert C. Dunbar,<sup>†\*</sup> Jeffrey D. Steill,<sup>‡</sup> Nicolas C. Polfer,<sup>#</sup> Giel Berden<sup>‡</sup> and Jos Oomens<sup>§</sup>; <sup>†</sup>*Chemistry Department, Case Western Reserve University, Cleveland, OH*, <sup>#</sup>*Chemistry Department, University of Florida, Gainesville, FL*, <sup>‡</sup>*FOM-Institute for Plasma Physics Rijnhuizen, NL-3439 MN Nieuwegein, The Netherlands*, <sup>§</sup>*University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands*
- 60 **In Situ Enrichment of Phosphopeptides on MALDI Plates Functionalized by Ambient Ion Landing;** Petr Pompach<sup>1</sup>, Lukas Krásný<sup>1,2</sup>, Marcela Strnadova<sup>1</sup>, Petr Novak<sup>1</sup>, Martin Strohal<sup>1</sup>, Vladimir Havlicek<sup>1</sup>, Frantisek Tureček<sup>3</sup>, Karel Lemr<sup>4</sup>, Oldrich Benada<sup>1</sup>, and Michael Volný<sup>1</sup>; <sup>1</sup>*Institute of Microbiology AS CR, v.v.i., Prague, Czech Republic*, <sup>2</sup>*Institute of Chemical Technology, Prague, Czech Republic*, <sup>3</sup>*Department of Chemistry, University of Washington, Seattle, WA* and <sup>4</sup>*Department of Analytical Chemistry, Palacky University, Olomouc, Czech Republic*
- 61 **Characterizing Self-Assembled Extracellular Matrix Fibrillar Films with TOF-SIMS;** Christopher R. Anderton, Kiran Bhadriraju, Frank W. DelRio, and Anne L. Plant ; <sup>a</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- 62 **PCA of TOF-SIMS Data to Elucidate Lipid Distribution Within Biological Membranes;** Christopher R. Anderton,<sup>a,b\*</sup> Bitva Vaezian,<sup>a</sup> Kaiyan Lou,<sup>a</sup> and Mary L. Kraft<sup>a</sup> ; <sup>a</sup>*School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, IL* and <sup>b</sup>*Current institution: National Institute of Standards and Technology, Gaithersburg, MD*
- 63 **Custom QIT Mass Spectrometer for Infrared Photodissociation Spectroscopy of Biomolecular Ions;** Corey N. Stedwell,<sup>†</sup> Kerim Gulyuz,<sup>†</sup> Nick C. Polfer<sup>†</sup>; <sup>†</sup>*Department of Chemistry, University of Florida, Gainesville, FL*

*Poster Topic*  
**Emerging Directions and Techniques**

- 64 **Vibrational Spectroscopy of  $b_2$  Fragment Ions from Peptides in the Hydrogen Stretching Region;** Kerim Gulyuz; Corey N. Stedwell; Da Wang; Nick C. Polfer; *University of Florida, Gainesville, FL*
- 65 **Analysis of Human SLOS Fibroblast Cholesterol and 7-Dehydrocholesterol via Silver Sputtering Laser Desorption Ionization – Ion Mobility – Mass Spectrometry and Computational Modeling;** Michal Kliman, Libin Xu, Sarah M. Stow, Ned A. Porter, John A. McLean; *Department of Chemistry, Vanderbilt University, Nashville, TN*