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ASMS2009 conference schedule for MICHAEL CHALMERS

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**Code:** - MOC am

**Time Slot/Poster Number:** 08:30 am    **Session:** Characterizing Protein-Protein Interactions

**Investigation of intact protein complexes and protein-protein interactions by native ion mobility and tandem mass spectrometry**

Esther Van Duijn; Arjan Barendregt; Charlotte Uetrecht; Kristina Lorenzen; Rebecca Rose; Glen Shoemaker; Albert J.R. Heck  
*Utrecht University, Utrecht , Netherlands*

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**Code:** - MOC am

**Time Slot/Poster Number:** 08:50 am    **Session:** Characterizing Protein-Protein Interactions

**Micelles protect ATP synthases from solution to gas phase and reveal novel protein interactions in membrane embedded subunits**

Carol Robinson; Min Zhou; Dijana Matak Vinkovic; Nina Morgner; Shoshanna Isaacson; Neslon Barrera  
*University of Cambridge, Cambridge, UK*

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**Code:** - MOC am

**Time Slot/Poster Number:** 09:10 am    **Session:** Characterizing Protein-Protein Interactions

**Transient protein interactions and ligand exchange between transporters and receptors: MS study of retinoic acid delivery to RAR by CRABP**

Virginie Sjoelund; Igor A. Kaltashov  
*University of Massachusetts, Amherst , MA*

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**Code:** - MOC am

**Time Slot/Poster Number:** 09:30 am    **Session:** Characterizing Protein-Protein Interactions

**Comprehensive Structural Mass Spectrometry for the Identification of Assembly Interactions in an HIV-1 Capsid Mutant Protein**

Lisa Jones<sup>1</sup>; Hao Zhang<sup>1</sup>; Michael L. Gross<sup>1</sup>; Peter Prevelige<sup>2</sup>  
<sup>1</sup>Washington University, St. Louis , MO; <sup>2</sup>University of Alabama, Birmingham, AL

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**Code:** - MOC am

**Time Slot/Poster Number:** 09:50 am    **Session:** Characterizing Protein-Protein Interactions

**New Approaches for Efficient Chemical Cross-linking of Proteins and Protein Complexes**

Julian Mintseris; Steven Gygi  
*Harvard Medical School, Boston , MA*

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**Code:** - MOC am

**Time Slot/Poster Number:** 10:10 am    **Session:** Characterizing Protein-Protein Interactions

**Assembly and stability of native and modified Shiga toxins investigated by ES-MS**

Elena Kitova<sup>1</sup>; George L Mulvey<sup>2</sup>; Tanis Dingle<sup>2</sup>; Thomas P Griener<sup>2</sup>; Glen D Armstrong<sup>2</sup>; John Klassen<sup>1</sup>  
<sup>1</sup>University of Alberta, Edmonton , Canada ; <sup>2</sup>University of Calgary, Calgary, Alberta

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Code: - MPB

Time Slot/Poster Number: 065 Session: Bioinformatics: Quantification

**Formulation of a MySQL database and Query toolset to extract complex metabolic information from a natural microbial consortia.**

Nathan C. Verberkmoes<sup>1</sup>; Brian Dill<sup>1</sup>; Brian Thomas<sup>2</sup>; Denise Schmoyer<sup>1</sup>; Manesh Shah<sup>1</sup>; Vincent Deneff<sup>2</sup>; Paul Wilmes<sup>2</sup>; Patricia Carey<sup>1</sup>; Steve Singer<sup>3</sup>; Korin Wheeler<sup>3</sup>; Michael Thelen<sup>3</sup>; Robert Hettich<sup>1</sup>

<sup>1</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>Lawrence Livermore National Laboratory, Livermore, CA

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Code: - MPL

Time Slot/Poster Number: 286 Session: Proteomics: PTM Determination (Method Development)

**An Integrated Bottom-up and Top-down Characterization of Metalloproteins and Protein Molecular Forms in the Extracellular Fraction of Extremophilic Microbial Communities**

Brian K. Erickson<sup>1</sup>; Steven Singer<sup>2</sup>; Korin Wheeler<sup>2</sup>; Nathan C. Verberkmoes<sup>3</sup>; Manesh Shah<sup>3</sup>; Michael Thelen<sup>2</sup>; Jill Banfield<sup>4</sup>; Robert Hettich<sup>3</sup>

<sup>1</sup>University of Tennessee - Oak Ridge National Lab, Knoxville, TN; <sup>2</sup>Lawrence Livermore National Laboratory, Livermore, CA; <sup>3</sup>Oak Ridge Nat'l Lab, Oak Ridge, TN; <sup>4</sup>University of California - Berkeley, Berkeley, CA

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Code: - MPL

Time Slot/Poster Number: 297 Session: Proteomics: PTM Determination (Method Development)

**Characterizing Protein Post-translational Modifications in Cellulose-degrading Bacteria by a Combined CAD and ETD Approach**

Andrew B. Dykstra<sup>1,2</sup>; Richard J. Giannone<sup>2</sup>; Adriane Lochner<sup>2</sup>; Kelsey D. Cook<sup>1</sup>; Robert L. Hettich<sup>2</sup>

<sup>1</sup>University of Tennessee, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN

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Code: - MPQ

Time Slot/Poster Number: 394 Session: Immunology

**Antibody-Antigen Binding Affinity Measurement Using HD Exchange and Dilution Strategy**

Tingting Tu<sup>1</sup>; Don L. Rempel<sup>1</sup>; Alina Petre<sup>2</sup>; Michael Przybylski<sup>2</sup>; Michael L. Gross<sup>1</sup>

<sup>1</sup>Washington University in St. Louis, Saint Louis, MO; <sup>2</sup>University of Konstanz, Konstanz, GERMANY

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Code: - TOA am

Time Slot/Poster Number: 09:50 am Session: Mass Spectrometry and Biofuels

**Identification of the extracellular cellulolytic enzymes in thermophilic bacteria that are important for microbial cellulose degradation to bioethanol.**

Richard J. Giannone<sup>1</sup>; Adriane Lochner<sup>1</sup>; Andrew Dykstra<sup>1,2</sup>; Martin Keller<sup>1</sup>; James G. Elkins<sup>1</sup>; Robert Hettich<sup>1</sup>

<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>The University of Tennessee, Knoxville, TN

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Code: - TOC am

Time Slot/Poster Number: 08:30 am Session: Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Mass Spectrometry-Based Approaches for Monitoring Protein-Ligand Interactions: An Overview**

Lars Konermann; Jingxi Pan; Brian Boys

The University of Western Ontario, London, ON, Canada

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Code: - TOC am

Time Slot/Poster Number: 08:50 am Session: Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Hydroxyl radical footprinting of CCL5-chondroitin sulfate complex reveals both the binding interface and a ligand-induced conformational change**

Caroline Watson; Fei Yu; James Prestegard; Joshua S. Sharp  
*Complex Carbohydrate Research Center/UGA, Athens, GA*

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**Code:** - TOC am

**Time Slot/Poster Number:** 09:10 am **Session:** Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Ligand Binding and Conformational Flexibility of Ribosomes**

William Running; James P. Reilly  
*Indiana University, Bloomington, IN*

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**Code:** - TOC am

**Time Slot/Poster Number:** 09:30 am **Session:** Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Design and Application of Novel Cross-Linking Reagents for Mapping Protein-Protein Interactions**

Danielle Vellucci; Lan Huang; Scott Rychnovsky  
*University of California, Irvine, CA*

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**Code:** - TOC am

**Time Slot/Poster Number:** 09:50 am **Session:** Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Investigation of VDR modulator interactions with the full length VDR/RXR $\alpha$  nuclear receptor complex by HDX-MS**

Jun Zhang; Michael Chalmers; Bruce Pascal; Patrick Griffin  
*The Scripps Research Institute, Scripps Florida, Jupiter, FL*

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**Code:** - TOC am

**Time Slot/Poster Number:** 10:10 am **Session:** Characterizing Protein-Ligand Interactions with Mass Spectrometry

**Thermodynamic Analysis of Chaperone-Substrate Complexes**

Ying Xu<sup>1</sup>; Sebastian Schmitt<sup>2</sup>; Liangjie Tang<sup>3</sup>; Ursula Jakob<sup>2</sup>; Michael C. Fitzgerald<sup>1</sup>  
<sup>1</sup>Duke University, Durham, NC; <sup>2</sup>University of Michigan, Ann Arbor, MI; <sup>3</sup>ExSAR Corporation, Monmouth Junction, NJ

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**Code:** - TPE

**Time Slot/Poster Number:** 126 **Session:** Proteomics: New Approaches

**Use of proteinase K to improve resolution in hydrogen/deuterium exchange mass spectrometry**

John Venable; Linda Okach; William Scuba; Ansgar Brock  
*Genomics Institute for the Novartis Research Found, San Diego, CA*

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**Code:** - TPH

**Time Slot/Poster Number:** 215 **Session:** Ion Mobility I

**Evidence for Promotion of H/D Exchange During Transitions Between Conformations of the [M+11H]<sup>11+</sup> State of Ubiquitin**

Brian C. Bohrer; Natalya Atlasevich; David E. Clemmer  
*Indiana University, Bloomington, IN*

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**Code:** - TPN

**Time Slot/Poster Number:** 332 **Session:** LC/MS Sample Preparation

**Assessing the variability of peptide peak areas in online pepsin digestion**

Joomi Ahn<sup>1</sup>; Martha Stapels<sup>1</sup>; Keith Fadgen<sup>1</sup>; John R. Engen<sup>2</sup>  
<sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Northeastern University, Boston, MA

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**Code:** - TPS

**Time Slot/Poster Number:** 424 **Session:** Protein Conformation I

**Characterization of a Microfabricated Electrospray Ionization (ESI) Device for Solution-Phase H/D Exchange in Non-Denaturing Media**

Abdullah H. Al-Fdeilat; Behrooz Zekavat; Scott D. Collins; Rosemary Smith; Touradj Solouki  
*University of Maine, Orono, ME*

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Code: - TPS

Time Slot/Poster Number: 425      Session: Protein Conformation I

**Investigation of rapid two-dimensional peptic peptide fractionation for HD exchange by nano-LC MALDI**

Wayne Chou; Nicholas Sam-Soon; Tom Poulos; Paul Gershon  
*UC-Irvine, Irvine, CA*

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Code: - TPS

Time Slot/Poster Number: 426      Session: Protein Conformation I

**Reduced back-exchange by modified RPLC mobile phase separation of proteolytic peptides for MS analysis of H/D exchange of solution-phase proteins**

Santosh G Valeja<sup>1,2</sup>; Mark R. Emmett<sup>1,2</sup>; Alan G. Marshall<sup>1,2</sup>  
<sup>1</sup>Nat'l High Magnetic Field Lab, Tallahassee, FL; <sup>2</sup>Florida State university, Tallahassee, FL

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Code: - TPS

Time Slot/Poster Number: 427      Session: Protein Conformation I

**H/D Exchange Combined with Top-Down Electron Capture Dissociation for Protein Complex Structural Characterization: Development and Early Results**

Magalie Duchateau; Charlotte Boisseau; Julia Chamot-rooke; Guillaume Van Der Rest  
*Ecole Polytechnique, Palaiseau, France*

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Code: - TPS

Time Slot/Poster Number: 428      Session: Protein Conformation I

**Tandem MS with a Label Reduction Strategy Enables a Proteomics Approach to H/DX Experiments**

Andrew Percy; David Schriemer  
*University of Calgary, Calgary, Canada*

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Code: - TPS

Time Slot/Poster Number: 429      Session: Protein Conformation I

**DEUTERIUM EXCHANGE MASS SPECTROMETRY USING A SEMIAUTOMATIC INTERFACE FOR DATA ACQUISITION AND AUTOMATIC DATA ANALYSIS AND REPORTING.**

Maria T. Villar; Danny E. Miller; Aron W. Fenton; Antonio Artigues  
*University of Kansas Medical Center, Kansas City, KS*

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Code: - TPS

Time Slot/Poster Number: 430      Session: Protein Conformation I

**Towards a standardized approach in presenting hydrogen-deuterium exchange mass spectrometry (HDX MS) data in comparability studies of biopharmaceutical products**

Cedric Bobst<sup>1</sup>; Rinat Abzalimov<sup>1</sup>; Damian Houde<sup>2,3</sup>; Marek Kloczewiak<sup>2</sup>; Steven A. Berkowitz<sup>2</sup>; John R. Engen<sup>3</sup>; Igor A. Kaltashov<sup>1</sup>  
<sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Biogen Idec, Inc., Cambridge, MA; <sup>3</sup>Northeastern University, Boston, MA

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Code: - TPS

Time Slot/Poster Number: 431      Session: Protein Conformation I

**ESI-MS Identifies Protein Oxidation as Major Contributor to Irreversible Thermal Denaturation**

Jenna-Jiangjiang Liu; Lars Konermann  
*Univ. of Western Ontario, London, ON*

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Code: - TPS

Time Slot/Poster Number: 432 Session: Protein Conformation I

**A new approach to assessing conformational stability and functional competence of protein therapeutics using mass spectrometry**

Cedric Bobst<sup>1</sup>; Rinat Abzalimov<sup>1</sup>; Damian Houde<sup>2</sup>; Steven A. Berkowitz<sup>2</sup>; Rohin Mhatre<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>

<sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Biogen Idec, Inc., Cambridge, MA

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Code: - TPS

Time Slot/Poster Number: 433 Session: Protein Conformation I

**Protein Equilibrium Population Snapshot (PEPS) MS method for Measuring Protein Folding Energies using H/D exchange and Oxidation of Methionine.**

Rohana Liyanage; Nagarjuna Devarapalli; Latisha M. Puckett; N.H. Phan; Joel A. Starch; Jennifer Gidden; Wesley E. Stites; Jackson O. Lay

University of Arkansas, Fayetteville, AR

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Code: - TPS

Time Slot/Poster Number: 434 Session: Protein Conformation I

**His-HDX Method to Probe the Microenvironment of Histidine Residues in Escherichia coli Dihydrofolate Reductase**

Masaru Miyagi; Chris Dealwis

Case Western Reserve University, Cleveland, OH

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Code: - TPS

Time Slot/Poster Number: 435 Session: Protein Conformation I

**Metal-catalyzed hydrogen/deuterium exchange and MS as a new way to determine metal-protein binding sites**

Adam M. Graichen; Richard Vachet

University of Massachusetts, Amherst, MA

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Code: - TPS

Time Slot/Poster Number: 436 Session: Protein Conformation I

**Structural and dynamic investigation of *umuD* gene products by hydrogen exchange mass spectrometry**

Jing Fang; Penny J. Beuning; John R. Engen

Northeastern University, Boston, MA

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Code: - TPS

Time Slot/Poster Number: 437 Session: Protein Conformation I

**Differences in structural dynamics of Factor VIII and Lactadherin C2 domains in relation to membrane binding employing DXMS analysis.**

Dennis Pantazatos<sup>3</sup>; Virgil Woods, Jr.<sup>5</sup>; Gary E. Gilbert<sup>1,2</sup>; Chris Gessner<sup>4</sup>

<sup>1</sup>VA Boston Health Care System, West Roxbury, MA; <sup>2</sup>Brigham and Women's Hospital, Boston, MA; <sup>3</sup>Harvard Medical School, Boston, MA; <sup>4</sup>Ohio State University, Columbus, OH; <sup>5</sup>University of California, La Jolla, CA

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Code: - TPS

Time Slot/Poster Number: 438 Session: Protein Conformation I

**The interaction of myristoylated HIV Nef with N-myristoyltransferase-1 as determined by hydrogen exchange mass spectrometry**

Chris Morgan<sup>1</sup>; Purushottam S. Narute<sup>2</sup>; Brian V. Miglionico<sup>1</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>

<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA

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Code: - TPS

Time Slot/Poster Number: 439 Session: Protein Conformation I

**Conformational Dynamics of the Transcription Regulator VraR are Modulated by Phosphorylation: A Hydrogen/Deuterium Exchange ESI-MS Study**

Yu-Hong Liu<sup>1</sup>; Antoaneta Belcheva<sup>2</sup>; Dasantila Golemi-Kotra<sup>2</sup>; Lars Konermann<sup>1</sup>  
<sup>1</sup>The University of Western Ontario, London, Canada; <sup>2</sup>York University, Toronto, Canada

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Code: - TPS

Time Slot/Poster Number: 440 Session: Protein Conformation I

**HIV-1 Vif conformation upon phosphorylation by MAPK and its implications in Elongin-BC binding**

Sean R. Marcisin; John R. Engen  
Northeastern University, Boston, MA

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Code: - TPS

Time Slot/Poster Number: 441 Session: Protein Conformation I

**Post-translational modifications alter intact IgG1 conformation and influence Fc-gamma-RIII binding**

Damian Houde<sup>1,2</sup>; Steven Berkowitz<sup>1</sup>; John R. Engen<sup>2</sup>  
<sup>1</sup>Biogen Idec, Inc., Cambridge, MA; <sup>2</sup>Northeastern University, Boston, MA

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Code: - TPS

Time Slot/Poster Number: 442 Session: Protein Conformation I

**Protein dynamics of Peroxiredoxins studied by Hydrogen/Deuterium Exchange Mass Spectrometry**

Sasidhar N Nirudodhi; Claudia Maier  
Oregon State University, Corvallis, OR

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Code: - TPS

Time Slot/Poster Number: 443 Session: Protein Conformation I

**Dynamic studies and structural delineation of truncated human cardiac troponin using HDX.**

Dev Kowlessur; Larry Tobacman  
University of Illinois, Chicago, IL

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Code: - TPS

Time Slot/Poster Number: 444 Session: Protein Conformation I

**Isotopic Depletion for the Structural Mapping of the Troponin Complex by Hydrogen/Deuterium Exchange Combined with FT-ICR Mass Spectrometry**

George M. Bou-assaf<sup>1,2</sup>; Jean E. Chamoun<sup>2,3</sup>; Mark R. Emmett<sup>1,2</sup>; Piotr G. Fajer<sup>2,4</sup>; Alan G. Marshall<sup>1,2</sup>  
<sup>1</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>2</sup>NHMFL/FSU, Tallahassee, FL; <sup>3</sup>Department of Chemistry, Macquarie University, Sydney, Australia; <sup>4</sup>Institute of Molecular Biophysics / FSU, Tallahassee, FL

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Code: - TPS

Time Slot/Poster Number: 445 Session: Protein Conformation I

**How Do the Four Keys (Ca<sup>2+</sup>) Change the World? A PLIMSTEX Study of Troponin C**

Richard Yu-cheng Huang; Don L. Rempel; Michael L. Gross  
Washington University, St. Louis, MO

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Code: - TPS

Time Slot/Poster Number: 446 Session: Protein Conformation I

**Accelerated Protein Folding due to Chaperone Action is Revealed by SUPREX.**

Stefan Esswein<sup>1</sup>; Hannah Florance<sup>2</sup>; Perdita Barran<sup>2</sup>  
<sup>1</sup>University of Edinburgh, Edinburgh, United Kingdom; <sup>2</sup>The University of Edinburgh, Edinburgh, UNITED KINGDOM

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Code: - TPS

Time Slot/Poster Number: 447 Session: Protein Conformation I

**Analysis of Histone Dynamics in the Higher Order Folding of Nucleosome Arrays Using Hydrogen/Deuterium Exchange Coupled to Mass Spectrometry**

Tanya Panchenko<sup>1</sup>; Sandya Ajith<sup>1</sup>; Mike Resch<sup>2</sup>; Jeffrey C. Hansen<sup>2</sup>; Ben E. Black<sup>1</sup>  
<sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Colorado State University, Fort Collins, Colorado*

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Code: - TPS

Time Slot/Poster Number: 448      Session: Protein Conformation I

**Structural mass spectrometry of the  $\alpha\beta$ -tubulin dimer supports a revised model of microtubule assembly**

Melissa J. Bennett<sup>1</sup>; John Chik<sup>1</sup>; Gordon Slys<sup>1</sup>; Tyler Luchko<sup>2</sup>; Dan L. Sackett<sup>3</sup>; David Schriemer<sup>1</sup>

<sup>1</sup>*University of Calgary, Calgary, AB*; <sup>2</sup>*Cross Cancer Institute, Edmonton, Canada*; <sup>3</sup>*National Institutes of Health, Bethesda, MD*

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Code: - TPS

Time Slot/Poster Number: 449      Session: Protein Conformation I

**Allosteric effects in the Abl kinase upon inhibitor binding**

ROXANA E. IACOB<sup>1,3</sup>; Jianming Zhang<sup>2</sup>; Nathanael S. Gray<sup>2</sup>; John R. Engen<sup>1,3</sup>

<sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Dana-Farber Cancer Institute, Harvard Medical, Boston, MA*; <sup>3</sup>*Barnett Institute, Boston, MA*

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Code: - TPS

Time Slot/Poster Number: 450      Session: Protein Conformation I

**Identification of an Allosteric Pathway in the Regulation of  $\alpha$ -Isopropylmalate Synthase from Mycobacterium Tuberculosis by Solution-phase H/D Exchange FT-ICR MS**

Mark R. Emmett<sup>1</sup>; Hui-Min Zhang<sup>1</sup>; Patrick A. Frantom<sup>2</sup>; John S. Blanchard<sup>2</sup>; Alan G. Marshall<sup>1</sup>

<sup>1</sup>*Nat'l High Magnetic Field Lab/Florida State Univ., Tallahassee, FL*; <sup>2</sup>*Albert Einstein College of Medicine, Bronx, NY*

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Code: - TPS

Time Slot/Poster Number: 451      Session: Protein Conformation I

**Folding of the protein Cex in solution and in the gas phase studied by hydrogen/deuterium exchange**

Peran Terrier; D. J. Douglas

*University of British Columbia, Vancouver, BC*

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Code: - TPS

Time Slot/Poster Number: 452      Session: Protein Conformation I

**Investigation of transferrin/transferrin receptor interaction by hydrogen-deuterium exchange mass spectrometry (HDX MS)**

Cedric Bobst<sup>1</sup>; Anne B. Mason<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>

<sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*University of Vermont Medical School, Burlington, VT*

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Code: - TPS

Time Slot/Poster Number: 453      Session: Protein Conformation I

**Study of the Conformation of Myoglobin Adsorbed on Nanoparticles with Hydrogen/Deuterium Exchange Mass Spectrometry**

Yaoling Long; David Barber; John R. Eyler

*University of Florida, Gainesville, FL*

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Code: - TPS

Time Slot/Poster Number: 454      Session: Protein Conformation I

**Hydrogen/Deuterium Exchange analysis of RXR-rexinoid interactions in the presence and absence of coactivator GRIP-1**

LeeAnn J. Boerma<sup>1</sup>; Gang Xia<sup>1</sup>; Cheng Qui<sup>1</sup>; Donald D. Muccio<sup>1</sup>; Matthew B. Renfrow<sup>2</sup>

<sup>1</sup>*UAB at Birmingham, Birmingham, AL*; <sup>2</sup>*University of Alabama at Birmingham, Birmingham, AL*

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Code: - TPS

Time Slot/Poster Number: 455      Session: Protein Conformation I

**Probing the effects of GTP hydrolysis state on the conformation of RhoA using HDX MS**

Madonna-Lily Choi; Michael P. Walsh; John K. Chik  
University of Calgary, Calgary, Canada

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**Code:** - TPS

**Time Slot/Poster Number:** 456    **Session:** Protein Conformation I

**Probing Host-Guest Complex Formation Between Cyclodextrins and Pharmaceutical Drugs Using Hydrogen-Deuterium Exchange.**

Adedamola Onipede; Christian Granados; Jon Robinson; Xiomara Soto; David Sierra; Dil Ramanathan  
Kean University, Union, NJ

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**Code:** - TPT

**Time Slot/Poster Number:** 459    **Session:** Non-Covalent Interactions I

**Enhanced stoichiometry measurements of heterogeneous sub-MDa protein assemblies by tandem MS: elucidation of subunit exchange mechanism in GroEL**

Rinat Abzalimov<sup>1</sup>; Sarah C. Wehri<sup>2</sup>; George H. Lorimer<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>  
<sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>University of Maryland College Park, College Park, MD

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**Code:** - TPW

**Time Slot/Poster Number:** 541    **Session:** Proteomics: Systems Biology

**Shotgun Proteomic Analysis of a Model 7-member Human Gut Microbiota created in Gnotobiotic Mice**

Alison L. Russell<sup>1,2</sup>; Nathan C. Verberkmoes<sup>2</sup>; Nathan McNulty<sup>3</sup>; Manesh Shah<sup>2</sup>; Jeffrey Gordon<sup>3</sup>; Robert Hettich<sup>2</sup>  
<sup>1</sup>Genome Sciences & Technology, UT-Knoxville, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>Center for Genome Sciences, Washington University, St. Louis, MO

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**Code:** - TOG pm

**Time Slot/Poster Number:** 2:30 pm    **Session:** HDX for Protein Structure and Folding

**Structure of lipid-free and lipid-bound human apolipoprotein A-I by hydrogen-deuterium exchange analyzed by mass spectrometry**

Palaniappan S Chetty<sup>1</sup>; Michael C Phillips<sup>1</sup>; Lund-Katz S<sup>1</sup>; Leland Mayne<sup>1</sup>; David Stranz<sup>2</sup>; Walter Englander<sup>1</sup>  
<sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Sierra Analytics, Inc., Modesto, CA

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**Code:** - TOG pm

**Time Slot/Poster Number:** 2:50 pm    **Session:** HDX for Protein Structure and Folding

**On the conformation of HIV-1 Nef from various viral strains**

Thomas E. Wales<sup>1</sup>; Lori Emert-Sedlak<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>  
<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA

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**Code:** - TOG pm

**Time Slot/Poster Number:** 3:10 pm    **Session:** HDX for Protein Structure and Folding

**Insight into the Escherichia coli L7/L12 Ribosomal Stalk Complex from Hydrogen Exchange Mass Spectrometry**

Stephanie Deroo<sup>1</sup>; Yuliya Gordiyenko<sup>1</sup>; Carol Robinson<sup>2</sup>  
<sup>1</sup>Cambridge University, Cambridge, United Kingdom; <sup>2</sup>University of Cambridge, Cambridge, UNITED KINGDOM

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**Code:** - TOG pm

**Time Slot/Poster Number:** 3:30 pm    **Session:** HDX for Protein Structure and Folding

**Conformational and Functional Effect of Posttranslational Modifications on sRAGE Protein by Solution-Phase H/D Exchange FT-ICR Mass Spectrometry**

Hui-Min Zhang<sup>1</sup>; Shaun Mcloughlin<sup>2</sup>; Huan He<sup>1</sup>; Carol Nilsson<sup>3</sup>; Mark R. Emmett<sup>1</sup>; Alan G. Marshall<sup>1</sup>  
<sup>1</sup>Nat'l High Magnetic Field Lab/Florida State Univ., Tallahassee, FL; <sup>2</sup>Abbott Laboratories, Abbott Park, IL; <sup>3</sup>Pfizer, Inc., San Diego, CA

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Code: - TOG pm

Time Slot/Poster Number: 3:50 pm Session: HDX for Protein Structure and Folding

**Amyloidogenic beta-2-microglobulin transiently populates a long-lived unfolded state**

Thomas J.d. Jorgensen<sup>1</sup>; Lei Cheng<sup>2</sup>; Anna Jansson<sup>4</sup>; Niels H.H. Heegaard<sup>3</sup>

<sup>1</sup>University of Southern Denmark, Odense M, Denmark; <sup>2</sup>Dept. Biochemistry & Molecular Biology, Odense M, DENMARK;

<sup>3</sup>Statens Serum Institut, Copenhagen, Denmark; <sup>4</sup>Sidec AB, Stockholm, Sweden

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Code: - TOG pm

Time Slot/Poster Number: 4:10 pm Session: HDX for Protein Structure and Folding

**Examination of electron-induced fragmentation of intact protein ions as a new tool in top-down HDX MS measurements**

Rinat Abzalimov<sup>1</sup>; Desmond Kaplan<sup>2</sup>; Michael Easterling<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>

<sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Bruker Daltonics, inc., Billerica, MA

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Code: - WPE

Time Slot/Poster Number: 131 Session: Proteomics: New Approaches

**Extending the dynamic range of proteome measurement in a natural microbial community with IEF protein fractionation and multidimensional LC-MS/MS.**

Brian D. Dill<sup>1</sup>; Paul Wilmes<sup>2</sup>; Vincent Deneff<sup>2</sup>; Manesh Shah<sup>1</sup>; Michael P. Thelen<sup>3</sup>; Brian Erickson<sup>1,4</sup>; Robert Hettich<sup>1</sup>; Jill F. Banfield<sup>2</sup>; Nathan C. VerBerkmoes<sup>1</sup>

<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>Pacific Northwest National Laboratory, West Richland, WA; <sup>4</sup>University of Tennessee, Knoxville, TN

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Code: - WPH

Time Slot/Poster Number: 201 Session: Ion Mobility II

**Hydrogen/Deuterium Exchange of Mobility Selected Ubiquitin Ions Using a High-Resolution Circular Ion Mobility Spectrometry Instrument in Ring-Down Mode**

Rebecca S. Glaskin; Samuel Merenbloom; David E. Clemmer  
*Indiana University, Bloomington, IN*

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Code: - WPL

Time Slot/Poster Number: 321 Session: Instrumentation: New Concepts

**Online bioaffinity-electrospray mass spectrometry: Combining molecular identification and bioaffinity quantification in biopolymer interactions**

Michael Przybylski<sup>1</sup>; Mihaela Dragusanu<sup>1</sup>; Stefan Slamnoi<sup>1</sup>; Alina Petre<sup>1</sup>; Tingting Tu<sup>2</sup>; Michael L. Gross<sup>2</sup>

<sup>1</sup>University of Konstanz, Konstanz, GERMANY; <sup>2</sup>Washington University, Saint Louis, MO

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Code: - WPR

Time Slot/Poster Number: 415 Session: Protein Conformation II

**AMOM: Investigational New Analytical Marker of Oxidation for Monoclonal Antibodies using RP-LC/MS, Peptide Maps and SPR**

John C. Le; Justin T. Paroski; Bernice Yeung; Byeong S. Chang  
*Symyx Technologies Inc., Camarillo, CA*

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Code: - WPR

Time Slot/Poster Number: 416 Session: Protein Conformation II

**Thermodynamic measurements of enzyme stabilities using H/D exchange and MALDI-TOF MS**

Cheng-Ying Lin; Yen-Peng Ho  
*National Dong Hwa University, Hualien, Taiwan*

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Code: - WPR

Time Slot/Poster Number: 417 Session: Protein Conformation II

**Ligand Binding to Cytochrome P450 46A1 as Assessed by Hydrogen – Deuterium Exchange and Mass Spectrometry**

Wei-Li Liao<sup>1</sup>; Nathan Dodder<sup>2</sup>; Natalia Mast<sup>3</sup>; Irina A Pikuleva<sup>3</sup>; Illarion V. Turko<sup>1</sup>

<sup>1</sup>Center for Advanced Research in Biotechnology, Rockville, MD; <sup>2</sup>NIST, Gaithersburg, MD; <sup>3</sup>Case Western Reserve University, Cleveland, OH

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Code: - WPR

Time Slot/Poster Number: 418 Session: Protein Conformation II

**Allosteric Networks and Regulation of Protein Kinase A: Amide H/D Exchange Mass Spectrometry Reveals Parallels between cAMP Binding and Phosphorylation**

Ganesh S. Anand<sup>1</sup>; Tanushree Bishnoi<sup>1</sup>; Susan Taylor<sup>2</sup>; Elizabeth Komives<sup>2</sup>

<sup>1</sup>National University of Singapore, Singapore, Singapore; <sup>2</sup>University of California, La Jolla, CA

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Code: - WPR

Time Slot/Poster Number: 419 Session: Protein Conformation II

**70S ribosomal-protein dynamics in translocation revealed by H/D exchange and mass spectrometry**

Tatsuya Yamamoto<sup>1</sup>; Yoshihiro Shimizu<sup>2</sup>; Takuya Ueda<sup>2</sup>; Yoshitsugu Shiro<sup>1</sup>

<sup>1</sup>RIKEN, Sayo-gun, Japan; <sup>2</sup>Grad. Sch. Frontier Sci., Univ. Tokyo, Kashiwa, Japan

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Code: - WPR

Time Slot/Poster Number: 420 Session: Protein Conformation II

**Two new tools for applying chromatographic retention data to the mass-identification of HDX peptides during HD-exchange experiments by nanoLC-MALDI**

Enrique Cauich; Paul Gershon  
UC-Irvine, Irvine, CA

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Code: - WPR

Time Slot/Poster Number: 421 Session: Protein Conformation II

**Combined ion mobility and rapid gas-phase deuterium labeling in a Synapt mass spectrometer for enhanced detection of protein conformations**

Kasper D. Rand<sup>1</sup>; James P. Murphy III<sup>2</sup>; Keith Fadgen<sup>2</sup>; John R. Engen<sup>1</sup>

<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Waters Corporation, Milford, MA

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Code: - WPR

Time Slot/Poster Number: 422 Session: Protein Conformation II

**Generation of Native Protein Ions and H/D Exchange in Liquid Sample Desorption Electrospray Ionization Mass Spectrometry (DESI-MS)**

Zhixin Miao; Hao Chen  
Ohio University, Athens, OH

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Code: - WPR

Time Slot/Poster Number: 423 Session: Protein Conformation II

**New developments to HD Desktop software for the data analysis of hydrogen exchange mass spectra**

Bruce Pascal; Michael Chalmers; Jun Zhang; Scott Busby; Patrick R. Griffin  
The Scripps Research Institute, Scripps Florida, Jupiter, FL

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Code: - WPR

Time Slot/Poster Number: 424 Session: Protein Conformation II

**Characterization of thermal unfolding in proteins using electrospray ionization time of flight mass spectrometry and top down fragmentation.**

Douglas Rehder; sabine paterson; David Hambly; Jaby Jacob; Michael J Treuheit; Bruce Kerwin; Himanshu Gadgil  
Amgen Inc., Seattle, WA

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Code: - WPR

Time Slot/Poster Number: 425 Session: Protein Conformation II

**IR Photodissociation Spectra of Gaseous Protein Ions: Hydrogen Bonding of Side-Chain Protonated Amino Groups is Unusually Strong**

Xianglei Kong<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Fred W. McLafferty<sup>1</sup>

<sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, AUSTRIA

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Code: - WPR

Time Slot/Poster Number: 426 Session: Protein Conformation II

**New ECD kinetic probes of the unfolding and folding of protein conformers after electrospray**

Sergio Castro<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Fred W. McLafferty<sup>1</sup>

<sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, AUSTRIA

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Code: - WPR

Time Slot/Poster Number: 427 Session: Protein Conformation II

**Fragmentation of Gas Phase Ions of Ubiquitin Produced from Different Solution Conformations in a 3D Ion Trap**

John Wright

Varian Inc., Wood Dale, IL

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Code: - WPR

Time Slot/Poster Number: 428 Session: Protein Conformation II

**Mass spectrometry-based studies of the Vancomycin resistance pathway in *Enterococcus faecalis***

Charlotte A. Scarff; Andrew M. Quigley; Adrian J. Lloyd; David I. Roper; James H. Scrivens

University of Warwick, Coventry, United Kingdom

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Code: - WPR

Time Slot/Poster Number: 429 Session: Protein Conformation II

**Development of mass spectrometry-based experimental strategies for detection and characterization of proteins with non-native disulfide bonds**

Adriana Zeledon; Igor A. Kaltashov

University of Massachusetts, Amherst, MA

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Code: - WPR

Time Slot/Poster Number: 430 Session: Protein Conformation II

**Computational Methods for Incorporation of Structural Mass Spectrometry Data in Structure Determination**

Xiaojing Zheng<sup>1</sup>; Robert M Vernon<sup>2</sup>; David Baker<sup>2</sup>; Mark Chance<sup>3</sup>

<sup>1</sup>Case Western Reserve Univ., Cleveland, OH; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Case Western Reserve Univ., Cleveland, OH

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Code: - WPR

Time Slot/Poster Number: 431 Session: Protein Conformation II

**MS Cleavable Crosslinker for Protein Interactions**

Billy Clifford-Nunn; Eric Simon; Philip Andrews

University of Michigan, Ann Arbor, MI

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Code: - WPR

Time Slot/Poster Number: 432 Session: Protein Conformation II

**"MALDI-MS3" analysis of CID-cleavable isotopically coded crosslinker TEABS.**

Jamie Thomas; Evgeniy Petrotchenko; Christoph Borchers

UVic-GBC Proteomics Centre, Victoria, Canada

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Code: - WPR

Time Slot/Poster Number: 433 Session: Protein Conformation II

**Probing the Electrostatic Surface Topology of Proteins Using Combinatorial Collision-Induced Dissociative Chemical Crosslinking Reagents and Mass Spectrometry Analysis**

Fan Liu; [Michael B. Goshe](#)  
NC State University, Raleigh , NC

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Code: - WPR

Time Slot/Poster Number: 434 Session: Protein Conformation II

**Structural proteomics revisited: a top-down approach to chemical crosslinking and protein interactions.**

[Giuseppe Infusini](#); Weiwei Tong; David H. Perlman; Roger Theberge; Catherine E. Costello  
Boston University School of Medicine, Boston, MA

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Code: - WPR

Time Slot/Poster Number: 435 Session: Protein Conformation II

**A Strategy for Efficient Identification of Chemically-Crosslinked Sites in Large Protein Complexes Using Label-Free LC-MS/MS Pattern Comparisons And Targeted MS/MS**

[Donghai Li](#)<sup>1</sup>; Sandra L. Harper<sup>1</sup>; Hsin-yao Tang<sup>1</sup>; David W. Speicher<sup>1,2</sup>  
<sup>1</sup>The Wistar Institute, Philadelphia , PA; <sup>2</sup>Wistar Institute, Philadelphia, PA

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Code: - WPR

Time Slot/Poster Number: 436 Session: Protein Conformation II

**Development of polyproline linked bifunctional crosslinkers as molecular rulers for the structural investigation of protein assemblies**

[Timothy Garrett Jr.](#); Kevin B. Turner; Daniele Fabris  
U. Maryland Baltimore County, Baltimore, MD

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Code: - WPR

Time Slot/Poster Number: 437 Session: Protein Conformation II

**Structure determination of proteins from the endoplasmic reticulum using chemical cross-linking, mass spectrometry and bioinformatics.**

[Morten Rasmussen](#)<sup>1</sup>; Tina Nielsen<sup>1</sup>; Gunnar Houen<sup>3</sup>; Juri Rappsilber<sup>2</sup>; Peter Hojrup<sup>1</sup>  
<sup>1</sup>BMB, University of Southern Denmark, Odense M , Denmark ; <sup>2</sup>Wellcome Trust Centre for Cell Biology, Edinburgh, UNITED KINGDOM; <sup>3</sup>Statens Serum Institut, Copenhagen, Denmark

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Code: - WPR

Time Slot/Poster Number: 438 Session: Protein Conformation II

**Use of N-terminal modification with isotopically coded reagents for selective identification of inter-peptide crosslinks**

[Jason Serpa](#); Evgeniy Petrotchenko; Christoph Borchers  
UVic-GBC Proteomics Centre, Victoria , Canada

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Code: - WPR

Time Slot/Poster Number: 439 Session: Protein Conformation II

**Crosslinking Techniques for Structural Studies of Large, Multi-chain Coagulation-related Proteins**

[Susan T. Lord](#)<sup>1</sup>; Maria Warren Hines<sup>2</sup>; Evgeniy Petrotchenko<sup>3</sup>; Carol E. Parker<sup>2</sup>  
<sup>1</sup>Department of Pathology & Lab.Medicine, UNC-CH, Chapel Hill, NC; <sup>2</sup>UNC-Duke Proteomics Center, UNC-CH, Chapel Hill, NC; <sup>3</sup>UVic-GBC Proteomics Centre, Victoria, BC

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Code: - WPR

Time Slot/Poster Number: 440 Session: Protein Conformation II

**Out-gel Digest Procedure for Protein Cross-linking Applications**

Ashley Cabecinha; Evgeniy Petrotchenko; Christoph Borchers  
*UVic-GBC Proteomics Centre, Victoria , Canada*

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Code: - WPR

Time Slot/Poster Number: 441 Session: Protein Conformation II

**Probability based Shotgun Approach for Cross-linking Sites Analysis by Mass Spectrometry**

Young Jin Lee  
*Iowa State University, Ames , IA*

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Code: - WPR

Time Slot/Poster Number: 442 Session: Protein Conformation II

**Characterization of  $\beta$ 2m Dimer Formation using Covalent Labeling, Bottom-Up, and Top-Down Strategies**

Vanessa Leah Mendoza<sup>1</sup>; Jonathan Wilson<sup>2</sup>; Desmond Kaplan<sup>2</sup>; Richard Vachet<sup>1</sup>  
<sup>1</sup>*University of Massachusetts, Amherst , MA*; <sup>2</sup>*Bruker Daltonics, Inc., Billerica, MA*

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Code: - WPR

Time Slot/Poster Number: 443 Session: Protein Conformation II

**Structural study of C3b-H complex using gamma and synchrotron irradiation coupled with semi-quantitative mass spectrometry**

Maxime Le Mignon<sup>1,2</sup>; Florence Gonnet<sup>1,2</sup>; Sebastien Brier<sup>1,2</sup>; Delphine Pflieger<sup>1,2</sup>; Bianca Sclavi<sup>3</sup>; Serge Pin<sup>4,5</sup>; Quentin Raffy<sup>4,5</sup>;  
Jean-Philippe Renault<sup>4,5</sup>; Régis Daniel<sup>1,2</sup>  
<sup>1</sup>*Université Evry-Val-d'Essonne, Evry, France*; <sup>2</sup>*CNRS UMR 8587, LAMBE, Evry, France*; <sup>3</sup>*CNRS UMR 8113, LBPA, Cachan, France*; <sup>4</sup>*CNRS URA 331 LCF, Gif-sur-Yvette, France*; <sup>5</sup>*CEA IRAMIS, Gif-sur-Yvette, France*

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Code: - WPR

Time Slot/Poster Number: 444 Session: Protein Conformation II

**Probing the Structure of Proinsulin by MS-Based Footprinting**

Janna Kiselar; Nelson B. Phillips; Mark R Chance; Michael A. Weiss  
*Case Western Reserve Univ, Cleveland , OH*

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Code: - WPR

Time Slot/Poster Number: 445 Session: Protein Conformation II

**Computational Methods for Examining Covalently Labeled Biomolecules using Structural Mass Spectrometry**

Parminder Kaur; Janna Kiselar; Mark Chance  
*Case Western Reserve Univ, Cleveland, OH*

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Code: - WPR

Time Slot/Poster Number: 446 Session: Protein Conformation II

**Characterizing the ATP-Induced Structural Changes of the N-terminal Domain of Pms1 by Oxidative Surface Mapping and Mass Spectrometry**

Allison N Schorzman<sup>1</sup>; Lalith Perera<sup>1</sup>; Lars C. Pedersen<sup>1</sup>; Jenny M. Cutalo<sup>2</sup>; Thomas A. Darden<sup>1</sup>; Thomas A. Kunkel<sup>1</sup>; Kenneth B. Tomer<sup>1</sup>  
<sup>1</sup>*NIEHS, RTP, NC*; <sup>2</sup>*FBI, Washington, D.C., DC*

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Code: - WPR

Time Slot/Poster Number: 447 Session: Protein Conformation II

**Autoantigen Structural Studies: Photolytic Oxidation and Chemical Modification Combined With Mass Spectrometry**

Jinglan Wang; James G Smedley III; Piotr J Bilski; Jeffrey F Kuhn; Kenneth B. Tomer; Leesa Deterding  
*NIEHS, Research Triangle Park , NC*

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Code: - WPR

Time Slot/Poster Number: 448 Session: Protein Conformation II

**Laser-Induced Oxidative Labeling of Proteins for Probing Folding Kinetics and Mechanisms**

Bradley B. Stocks; Lars Konermann  
*Univ. of Western Ontario, London, Canada*

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Code: - WPR

Time Slot/Poster Number: 449 Session: Protein Conformation II

**Structural Characterization of an Integral Membrane Protein by Oxidative Methionine Labeling and Mass Spectrometry**

Yan Pan  
*Uni. of Western Ontario, London, Canada*

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Code: - WPR

Time Slot/Poster Number: 450 Session: Protein Conformation II

**High sensitivity characterization of conformational differences in pharmaceutical proteins by rapid hydroxyl radical footprinting**

Caroline Watson<sup>1</sup>; Sergio G Tisminetzky<sup>2</sup>; Marshall W. Bern<sup>3</sup>; Joshua S. Sharp<sup>1</sup>  
<sup>1</sup>Complex Carbohydrate Research Center/UGA, Athens, GA; <sup>2</sup>Biotechnology Development Group, ICGEB, Trieste, Italy; <sup>3</sup>Palo Alto Research Center, Palo Alto, CA

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Code: - WPR

Time Slot/Poster Number: 451 Session: Protein Conformation II

**MS-based Carboxyl Group Protein Footprinting for Probing the Orientation of FMO Protein in Photosynthetic Bacterial Membranes**

Hao Zhang; Jianzhong Wen; Robert E. Blankenship; Michael L. Gross  
*Washington University, Saint Louis, MO*

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Code: - WPS

Time Slot/Poster Number: 458 Session: Non-Covalent Interactions II

**CLIP: A crosslinker for enrichment and confident identification of protein crosslinking sites by mass spectrometry**

Saiful M. Chowdhury<sup>1</sup>; Xiuxia Du<sup>2</sup>; Nikola Tolic<sup>1</sup>; Ashoka D. Polpitiya<sup>1</sup>; Ronald J. Moore<sup>1</sup>; John R. Cort<sup>1,3</sup>; Uljana M. Mayer<sup>1</sup>; Richard D. Smith<sup>1</sup>; Joshua N. Adkins<sup>1</sup>  
<sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of North Carolina, Charlotte, NC; <sup>3</sup>Washington State University, Tri-cities, Richland, WA

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Code: - WPS

Time Slot/Poster Number: 459 Session: Non-Covalent Interactions II

**Technology Development for Studying Transient Protein-Protein Interactions on Chromosomes: Identification of a Transient Acetyltransferase Interactome**

Samuel G. Mackintosh<sup>1</sup>; Sherri K. Smart<sup>1</sup>; Sean D. Taverna<sup>2</sup>; Ricky D. Edmondson<sup>1</sup>; Alan J. Tackett<sup>1</sup>  
<sup>1</sup>University of Arkansas for Medical Sciences, Little Rock, AR; <sup>2</sup>Johns Hopkins Medical School, Baltimore, MD

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Code: - WPS

Time Slot/Poster Number: 460 Session: Non-Covalent Interactions II

**Structural characterization of macromolecular protein complexes using chemical cross-linking and mass spectrometry**

Pragya Singh; Richard A. Pfuetzner; Scott A. Shaffer; Alexandre Panchaud; Eri Nakatani; Carlos E. Catalano; Samuel I. Miller; David R. Goodlett  
*University of Washington, Seattle, WA*

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Code: - WPS

Time Slot/Poster Number: 461 Session: Non-Covalent Interactions II

**Defining topological features of membrane proteins by electrospray ionization mass spectrometry.**

Lynsey N. Jones; Stephen A. Baldwin; Peter J. F. Henderson; Alison E. Ashcroft  
Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK

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**Code:** - WPS

**Time Slot/Poster Number:** 462      **Session:** Non-Covalent Interactions II

**Photo-crosslinking and Complementary Use of ESI and MALDI Mass Spectrometry to Map Interaction Sites between Transcriptional Activators and Mediator 15**

Bo Wang; Chinmay Majmudar; Anna Mapp; Kristina Hakansson  
University of Michigan, Ann Arbor, MI

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**Code:** - ThOA am

**Time Slot/Poster Number:** 08:50      **Session:** MS of Peptide and Protein Drugs

am

**Stability of protein therapeutics under near-physiological conditions: Conformation and dynamics of acid- $\beta$ -glucosidase**

Cedric Bobst<sup>1</sup>; John J. Thomas<sup>2</sup>; Paul Salinas<sup>2</sup>; Rinat Abzalimov<sup>1</sup>; Philip J. Savickas<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>  
<sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Shire HGT, Cambridge, MA

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**Code:** - ThOC am

**Time Slot/Poster Number:** 08:30      **Session:** Mass Spectrometry at the Interface between Chemistry and Biology

am

**Chemical biology approaches to understanding the regulation of nuclear receptors**

Michael J. Chalmers; Scott A. Busby; Ruben Garcia-Ordenez; Monica Istrate; Naresh Kumar; Scott Novick; Bruce D. Pascal; Jun Zhang; Patrick R. Griffin  
The Scripps Research Institute, Jupiter, FL

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**Code:** - ThOC am

**Time Slot/Poster Number:** 10:10      **Session:** Mass Spectrometry at the Interface between Chemistry and Biology

am

**Characterizing the partitioning between RNA regulatory structures in the Moloney murine leukemia virus using antisense LNAs**

Arie Hawkins; Daniele Fabris  
U. Maryland Baltimore County, Baltimore, MD

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**Code:** - ThOF am

**Time Slot/Poster Number:** 09:30      **Session:** Nucleic Acid MS

am

**Investigating higher-order structure of nucleic acids by IRMPD in FTICR mass spectrometry**

Joshua Wilhide; Katherine Kellersberger; Daniele Fabris  
U. Maryland Baltimore County, Baltimore, MD

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**Code:** - ThPA

**Time Slot/Poster Number:** 016      **Session:** Bioinformatics IV

**HeXicon++: Automating HDX Data Analysis**

Xinghua Lou<sup>1</sup>; Bernhard Y. Renard<sup>1</sup>; Marc Kirchner<sup>2</sup>; Ullrich Koethe<sup>1</sup>; Christian Graf<sup>3</sup>; Judith A.J. Steen<sup>2</sup>; Hanno Steen<sup>2</sup>; Matthias P. Mayer<sup>3</sup>; Fred Hamprecht<sup>1</sup>

<sup>1</sup>University of Heidelberg, Heidelberg, Germany; <sup>2</sup>Children's Hospital Boston / Harvard Medical, Boston, MA; <sup>3</sup>ZMBH, Heidelberg, GERMANY

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**Code:** - ThPA

**Time Slot/Poster Number:** 017      **Session:** Bioinformatics IV

**HDX by nanoLC-MALDI: Software for discovery of protein-wide correlations between peptide deuterium uptake data and structural or MD simulation parameters**

Vikram Bodicherla; Paul Gershon  
UC-Irvine, Irvine, CA

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Code: - ThPA

Time Slot/Poster Number: 029      Session: Bioinformatics IV

**Confident Identification of Single Amino Acid Polymorphisms by a Database-Searching Approach for Shotgun Proteomics**

Chongle Pan<sup>1</sup>; P. Douglas Hyatt<sup>1</sup>; Nathan C. Verberkmoes<sup>1</sup>; Jill F. Banfield<sup>2</sup>; Robert Hettich<sup>1</sup>  
<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of California, Berkeley, CA

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Code: - ThPA

Time Slot/Poster Number: 031      Session: Bioinformatics IV

**Investigating amino acid polymorphisms in a natural viral-microbial community by integrating high mass accuracy and de novo search algorithms.**

Patricia Carey<sup>1</sup>; Chongle Pan<sup>1</sup>; Manesh Shah<sup>1</sup>; Robert Hettich<sup>1</sup>; Mya Breitbart<sup>2</sup>; Jillian Banfield<sup>3</sup>; Nathan C. Verberkmoes<sup>1</sup>  
<sup>1</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>2</sup>University of South Florida, St. Petersburg, FL; <sup>3</sup>University of California, Berkeley, Berkeley, CA

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Code: - ThPK

Time Slot/Poster Number: 279      Session: Peptides: Post-Translational Modification I

**Molecular recognition specificity and bioaffinity quantification in biopolymer interaction of anti-3-nitrotyrosine antibody revealed by SAW-ESI-MS and PLIMSTEX**

Mihaela Dragusanu<sup>1</sup>; Brindusa-Alina Petre<sup>1</sup>; Tingting Tu<sup>2</sup>; Michael Gross<sup>2</sup>; Michael Przybylski<sup>1</sup>  
<sup>1</sup>University of Konstanz, Konstanz, Germany; <sup>2</sup>Washington University, St. Louis, Missouri

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Code: - ThPO

Time Slot/Poster Number: 389      Session: Microbial Analysis

**Investigating the Functional Activities and Cellular Processes of the Human Gut Microbiome by Multidimensional LC-MS/MS**

Robert Hettich<sup>1</sup>; Nathan C. Verberkmoes<sup>2</sup>; Alison Russell<sup>2</sup>; Manesh Shah<sup>1</sup>; Mark Lefsrud<sup>6</sup>; Adam Godzik<sup>3</sup>; Claire Fraser-Liggett<sup>5</sup>; Janet Jansson<sup>4</sup>  
<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>UT-Oak Ridge National Lab, Knoxville, TN; <sup>3</sup>Burnham Institute for Medical Research, La Jolla, CA; <sup>4</sup>Lawrence Berkeley National Lab, Berkeley, CA; <sup>5</sup>University of Maryland School of Medicine, Baltimore, MD; <sup>6</sup>McGill University, Quebec, Canada

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Code: - ThPP

Time Slot/Poster Number: 396      Session: Nucleic Acids

**Probing secondary and tertiary structures of ribonucleoprotein assemblies with synthetic deoxyribozymes**

Kevin B. Turner; Micheal German; Arie Hawkins; Alberto Berton; Daniele Fabris  
U. of Maryland, Baltimore County, Baltimore, MD

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Code: - ThPP

Time Slot/Poster Number: 414      Session: Nucleic Acids

**Probing RNA structure by selective 2' hydroxyl acylation analyzed by mass spectrometry (SHAMS)**

Alberto Berton<sup>1</sup>; Kevin B. Turner<sup>1</sup>; Robert G. Brinson<sup>2,3</sup>; John P. Marino<sup>3</sup>; Stuart F.J. Le Grice<sup>2</sup>; Daniele Fabris<sup>1</sup>  
<sup>1</sup>U. of Maryland, Baltimore County, Baltimore, MD; <sup>2</sup>National Cancer Institute, Frederick, MD; <sup>3</sup>Center for Advanced research in Biotechnology, Rockville, MD

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Code: - ThPR

Time Slot/Poster Number: 462      Session: Neuropeptides

**Using Deuterium Exchange Electrospray Mass Spectrometry to Evaluate Inhibitors of Amyloid- $\beta$  Oligomerization**

Zijuan Zhang; Jason J. Evans; Marrianna Torok  
*University of Massachusetts Boston, Boston , MA*

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**Code:** - ThPS

**Time Slot/Poster Number:** 479      **Session:** Proteins: General

**Utilization of a Flow Through Membrane Electrospray Probe for Online H/D Exchange ESI-MS**

Thomas P. White<sup>1</sup>; Juan Astorga-wells<sup>2</sup>; Tomas Bergman<sup>2</sup>; Hans Jornvall<sup>2</sup>; Thorleif Lavold<sup>3</sup>; Craig M. Whitehouse<sup>1</sup>

<sup>1</sup>*Analytica of Branford, Inc., Branford, CT*; <sup>2</sup>*Karolinska Institutet, Stockholm, SWEDEN*; <sup>3</sup>*Biomotif AB, Danderyd, SWEDEN*

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**Code:** - ThPS

**Time Slot/Poster Number:** 482      **Session:** Proteins: General

**Reconstituted nucleosomes containing recombinant human histones for mass spectrometry-based biophysical studies**

Sandya Ajith; Stacey Wood; Tanya Panchenko; Ben E. Black

*University of Pennsylvania, Philadelphia , PA*

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**Code:** - ThPS

**Time Slot/Poster Number:** 483      **Session:** Proteins: General

**Thermodynamic Analysis of Protein-Ligand Binding Interactions Using SPROX**

Graham M West; Stephanie Cordato; Michael C. Fitzgerald

*Duke University, Durham , NC*

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**Code:** - ThPS

**Time Slot/Poster Number:** 485      **Session:** Proteins: General

**Rapid, Isotope-Coded Method for Mapping Protein-Protein and Protein-Ligand Interactions**

Katina L Johnson; Matthew J Cuneo; Robert E London; Kenneth B Tomer; Jason G Williams

*NIEHS, NIH, DHHS, Research Triangle Park, NC*

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**Code:** - ThPT

**Time Slot/Poster Number:** 508      **Session:** Proteins: Membrane

**Development and Application of X-ray Footprinting (XF) for Structural Studies of Integral Membrane Proteins**

Sayan Gupta; Mark Chance

*Case Western Reserve Univ, Upton, NY*

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**Code:** - ThPV

**Time Slot/Poster Number:** 552      **Session:** Proteins: Modified

**Characterization of a Novel Amine Derivatization to Investigate the Structural Properties of Proteins by Mass Spectrometry.**

Lake N. Paul; Kenneth B. Tomer

*NIEHS, Raleigh , NC*

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**Code:** - ThPV

**Time Slot/Poster Number:** 559      **Session:** Proteins: Modified

**Optimizing the Kinetics of the Indirect Oxidation Pathway for an Electrochemistry-Based Protein Surface Mapping Pipeline**

Paul Abraham; Carlee McClintock; Jerry Parks; Vilmos Kertesz; Robert Hettich

*Oak Ridge National Laboratory, Oak Ridge, TN*

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**Code:** - ThPZ

**Time Slot/Poster Number:** 649      **Session:** Ion Molecule, Ion Electron, and Ion-Ion Reactions

**A Computational Investigation of the Gas Phase Hydrogen/Deuterium Exchange of Aspartic Acid and Arginine Containing Peptides**

Ning-shiuan Lee; Elaine M. Marzluff  
*Grinnell College, Grinnell , IA*

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**Code:** - ThPZ

**Time Slot/Poster Number:** 650      **Session:** Ion Molecule, Ion Electron, and Ion-Ion Reactions

**H/D Exchange and Computational Modeling of Serine-Containing Peptides in the Gas Phase**

Maya Lipert; Elaine M. Marzluff  
*Grinnell College, Grinnell , IA*

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**Code:** - ThPZ1

**Time Slot/Poster Number:** 661      **Session:** High Throughput Analysis/Robotics

**Efficiency and Throughput of an HDX- and Mass Spectrometry-Based Assay for Protein-Ligand Binding**

Patrick D. Dearmond; Erin D. Hopper; Graham M. West; Victor Anbalagan; Michael C. Fitzgerald  
*Duke University, Durham , NC*

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**Code:** - ThPZ1

**Time Slot/Poster Number:** 688      **Session:** High Throughput Analysis/Robotics

**A vortex cooled sample handling and processing system for automated H/D exchange mass spectrometry**

Yong Chen; Ansgar Brock  
*Novartis-GNF, San Diego , CA*

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