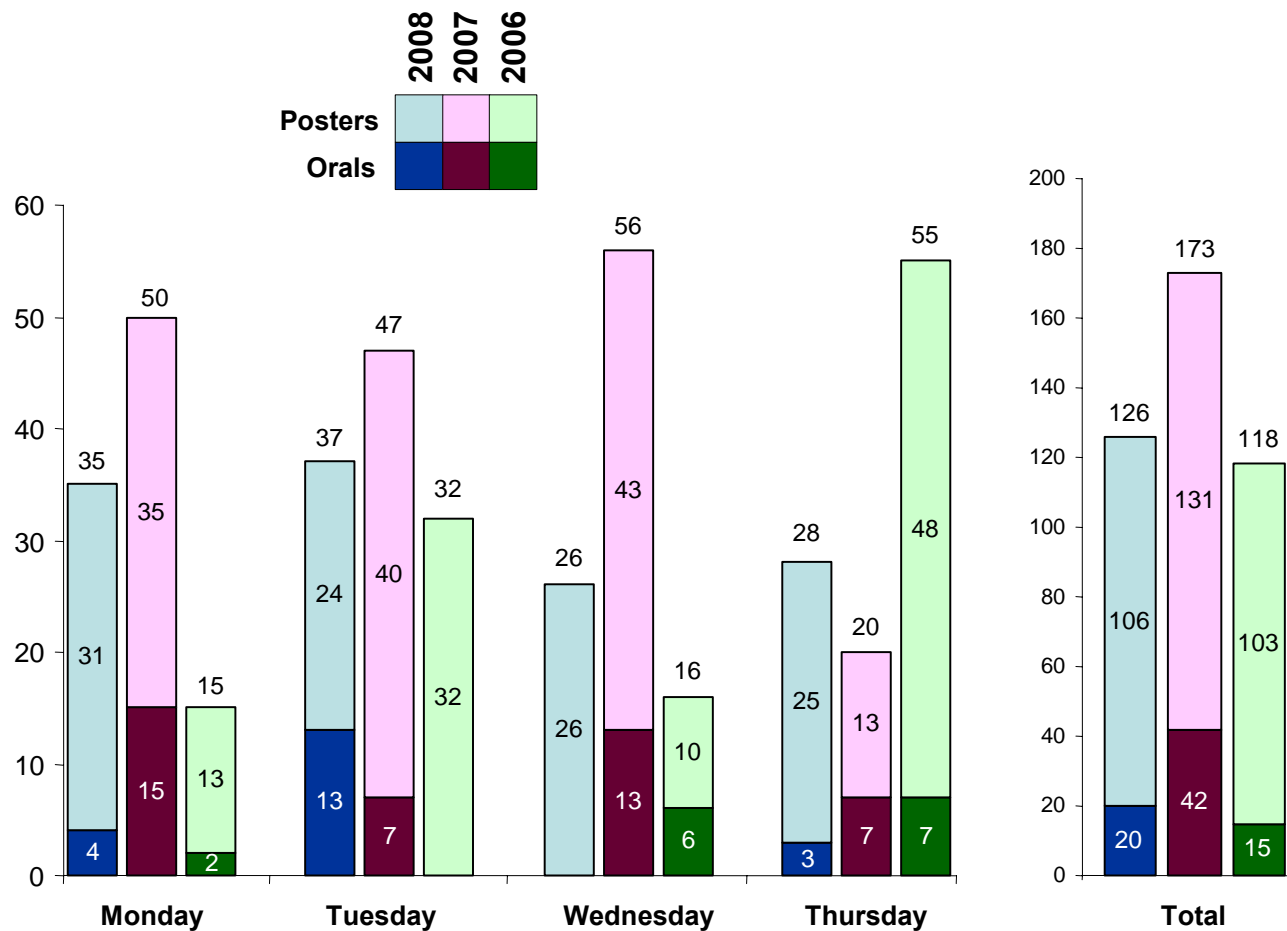


# ORALS & POSTERS SPECIFIC TO H/D EXCHANGE & COVALENT LABELING

ASMS 2008  
Denver, Colorado



List is as all-inclusive as possible. Please accept our apologies if something was missed  
Does not include iTRAQ, ICAT, 16O/18O, SILAC, HysTag, SeMet, or other quantitative labeling strategies, natural modifications

# MONDAY

**Code:** Monday - MOG pm

**Time Slot/Poster Number:** 2:30 pm

**Session:** Characterizing Protein-Ligand Interaction with Mass Spectrometry - Rooms 601-607

**Hydrogen / Deuterium exchange characterization of transmembrane signaling proteins**

MICHAEL CHALMERS<sup>3</sup>; Bruce Pascal<sup>3</sup>; Scott Novick<sup>3</sup>; Scott A. Busby<sup>3</sup>; Mark R Southern<sup>3</sup>; Ellen Chien<sup>1</sup>; Raymond C. Stevens<sup>1</sup>; David Szymkowski<sup>2</sup>; Patrick R. Griffin<sup>3</sup>; <sup>1</sup>TSRI, La Jolla, CA; <sup>2</sup>Xencor, Monrovia, CA; <sup>3</sup>The Scripps Research Institute - Florida, Jupiter, FL

**Code:** Monday - MOG pm

**Time Slot/Poster Number:** 3:10 pm

**Session:** Characterizing Protein-Ligand Interaction with Mass Spectrometry - Rooms 601-607

**Functional Consequences of Conformational Changes in the ClpP N-terminus and Ligand-driven ClpA Hexamer Formation: Structural MS of a Molecular Machine**

JEN BOHON<sup>1</sup>; Laura D. Jennings<sup>2</sup>; Christine M. Phillips<sup>2</sup>; Stuart Licht<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Upton, NY; <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA

**Code:** Monday - MOG pm

**Time Slot/Poster Number:** 3:30 pm

**Session:** Characterizing Protein-Ligand Interaction with Mass Spectrometry - Rooms 601-607

**Ion Mobility-Mass Spectrometry Reveals Subtle Stability Differences in Multi-protein Complex Ligand Assemblies**

Suk-joon Hyung; Brandon Ruotolo; Carol Robinson; *Department of Chemistry, University of Cambridge, Cambridge, UNITED KINGDOM*

**Code:** Monday - MOG pm

**Time Slot/Poster Number:** 3:50 pm

**Session:** Characterizing Protein-Ligand Interaction with Mass Spectrometry - Rooms 601-607

**A Protein-Ligand Binding Assay with Proteomic Potential**

MICHAEL C. FITZGERALD; Graham M. West; Victor Anbalagan; Liangjie Tang; *Duke University, Durham, NC*

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**Code:** Monday - MPB

**Time Slot/Poster Number:** 073

**Session:** APPI - Poster Hall

**Non-Uniform Isotope Patterns Produced by CID of Homogeneously Labeled Ubiquitin: Implications for Spatially-Resolved H/D Exchange Studies**

Peter L Ferguson<sup>2</sup>; LARS KONERMANN<sup>1</sup>; <sup>1</sup>Univ. of Western Ontario, London, CANADA; <sup>2</sup>Univ of Western Ontario, London, ON

**Code:** Monday - MPJ

**Time Slot/Poster Number:** 210

**Session:** Toxicology - Poster Hall

**Structure Elucidation of Formaldehyde-induced DNA-protein Cross-links by Mass spectrometry and NMR**

Kun Lu; Wenjie Ye; Li Zhou; Leonard Collins; Xian Chen; James Swenberg; *University of North Carolina, Chapel Hill, NC*

**Code:** Monday - MPMM

**Time Slot/Poster Number:** 334

**Session:** Peptides: Fragmentation - Poster Hall

**Fragment Structures in Collision-Induced Dissociation of Peptides Investigated by H/D Exchange**

XIAN CHEN; David H. Powell; Nicolas Polfer; *University of Florida, Gainesville, FL*

**Code:** Monday - MPMM

**Time Slot/Poster Number:** 350

**Session:** Peptides: Fragmentation - Poster Hall

**Gas phase fragmentation of peptides by MALDI in-source decay occurs with limited amide hydrogen (1H/2H) scrambling**

THOMAS J.D. JORGENSEN; Nicolai H Bache; Kasper Rand; Peter Roepstorff; *University of Southern Denmark, Odense M, DENMARK*

**Code:** Monday - MPP

**Time Slot/Poster Number:**

**Session:** Proteins: Crosslinking - Poster Hall

**Withdrawn**

LAU SENNELS<sup>1</sup>; Adam Belsom<sup>2</sup>; Mark Bradley<sup>2</sup>; Juri Rappsilber<sup>1</sup>; <sup>1</sup>Wellcome Trust Centre for Cell Biology, Edinburgh, United Kingdom; <sup>2</sup>School of Chemistry, University of Edinburgh, Edinburgh, United Kingdom

**Code:** Monday - MPP

**Time Slot/Poster Number:** 400

**Session:** Proteins: Crosslinking - Poster Hall

**A collection of novel isotopically-coded crosslinkers for structural proteomics.**

Evgeniy Petrotchenko; Jamie M. Thomas; Christoph Borchers; *UVic-GBC Proteomics Centre, Victoria, CANADA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 401

**Session:** Proteins: Crosslinking - Poster Hall

**Exploring CYP2B4-cytochrome b5 interaction by crosslinking reaction and mass spectrometry**

Miroslav Sulc<sup>1</sup>; Katerina Peslova<sup>1</sup>; Tomas Jecmen<sup>2</sup>; Petr Hodek<sup>2</sup>; Petr Novak<sup>1</sup>; <sup>1</sup>Institute of Microbiology, Prague, Prague 4, CZECH REPUBLIC; <sup>2</sup>Charles University, Faculty of Science, Prague 2, Czech Republic

**Code:** Monday - MPP

**Time Slot/Poster Number:** 402

**Session:** Proteins: Crosslinking - Poster Hall

**Multiplexed MS/MS methods and protein interaction identification**

Hye In Nam; Gerhard R. Munske; Li Yang; Haizhen Zhang; James E. Bruce; *Washington State University, Pullman, WA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 403

**Session:** Proteins: Crosslinking - Poster Hall

**Chemical Crosslinking and Chemical Modification Studies of LaSSB and Ro52, Autoantigens Associated with Sjogren's Syndrome**

LEESA DETERDING; Rachelle Bienstock; Kenneth B. Tomer; *NIEHS, RTP, NC*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 404

**Session:** Proteins: Crosslinking - Poster Hall

**Analysis of protein cross-linking by LC-MS/MS and a simple database search method**

Caifeng Zhao<sup>1</sup>; Daniel Henriquez<sup>2</sup>; Monica Roth<sup>3</sup>; Oscar Leon<sup>2</sup>; Haiyan Zheng<sup>1</sup>; <sup>1</sup>CABM, UMDNJ-RWJMS, Piscataway, NJ; <sup>2</sup>Programa de Virología, ICBM .University of Chile., Santiago, Chile; <sup>3</sup>Department of Biochemistry, UMDNJ-RWJMS, Piscataway, NJ

**Code:** Monday - MPP

**Time Slot/Poster Number:** 405

**Session:** Proteins: Crosslinking - Poster Hall

**Design and Evaluation of a Novel Homobifunctional Cross-linker with Selective Metal Dioxide-Based Enrichment Potential**

BO WANG; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 406

**Session:** Proteins: Crosslinking - Poster Hall

**Mining protein-protein interactions of proteins in Synechocystis sp. PCC 6803: novel chemical cross-linking and mass spectrometry**

CHUNXIANG ZHENG; Haizhen Zhang; Gerhard R. Munske; Xiaoting Tang; James E. Bruce; *Washington State University, Pullman, WA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 407

**Session:** Proteins: Crosslinking - Poster Hall

**Proteomics Analysis of Mammalian Cell Cultures for Biopharmaceutical Manufacturing**

Tyler Carlage<sup>1</sup>; Li Zang<sup>1</sup>; Yelena Lyubarskaya<sup>1</sup>; Marina Hincapie<sup>2</sup>; Rohin Mhatre<sup>1</sup>; William Hancock<sup>2</sup>; <sup>1</sup>Biogen Idec, Cambridge, MA; <sup>2</sup>Northeastern University, Boston, MA

**Code:** Monday - MPP

**Time Slot/Poster Number:** 409

**Session:** Proteins: Crosslinking - Poster Hall

**A new cross-linking strategy for exploring protein-protein interactions**

christian tagwerker; Danielle Vellucci; Ryan Benz; Pierre Baldi; Scott Rychnovsky; LAN HUANG; *University of California, Irvine, CA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 410

**Session:** Proteins: Crosslinking - Poster Hall

**Studying the Stepwise Progression of Formaldehyde Mediated Protein Crosslinking with Mass Spectrometry**

Judy Toews<sup>3</sup>; Jason Rogalski<sup>1</sup>; Juergen Kast<sup>2</sup>; *Biomedical Research Centr, Vancouver, CANADA*; <sup>2</sup>*University of British Columb, Vancouver, BC*; <sup>3</sup>*Biomedical Research Centre, Vancouver, BC*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 411

**Session:** Proteins: Crosslinking - Poster Hall

**Annexin A2/P11 interaction: New insights into annexin A2 tetramer structure by chemical crosslinking, high-resolution mass spectrometry, and computational modeling**

Daniela M. Schulz<sup>1</sup>; Stefan Kalkhof<sup>2</sup>; Andreas Schmidt<sup>5</sup>; CHRISTIAN H. IHLING<sup>2</sup>; Christoph Stingl<sup>6</sup>; Karl Mechtler<sup>3</sup>; Olaf Zschörnig<sup>4</sup>; Andrea Sinz<sup>2</sup>; <sup>1</sup>*Biotechnological-Biomedical Center, Leipzig, Germany*; <sup>2</sup>*Institute of Pharmacy, Halle, GERMANY*; <sup>3</sup>*Imp Research Institute of Mo, Vienna, AUSTRIA*; <sup>4</sup>*Institute for Medical Physics & Biophysics, Leipzig, Germany*; <sup>5</sup>*Cd Laboratory / Vienna, Vienna, AUSTRIA*; <sup>6</sup>*Institute of Moleculare Biotechnology, Vienna, AUSTRIA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 412

**Session:** Proteins: Crosslinking - Poster Hall

**Characterizing the 26S Proteasome Network in Yeast using a Quantitative In-Vivo Crosslinking Strategy and PPI Network Analysis**

Cortnie Guerrero<sup>1</sup>; Tijana Milenkovic<sup>1</sup>; Jeffrey J. Jones<sup>2</sup>; Natasa Przulj<sup>1</sup>; Peter Kaiser<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>*UC Irvine, Santa Ana, CA*; <sup>2</sup>*Applied Proteomics, Glendale, CA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 413

**Session:** Proteins: Crosslinking - Poster Hall

**Cross-Linking Analysis of Affinity-Purified Multi-Protein Complexes.**

Zhuo Chen; Morten Rasmussen; Salman Tahir; Sjaak van der Sar; Kevin G. Hardwick; Juri Rappsilber; *Wellcome Trust Centre for Cell Biology, Edinburgh, UNITED KINGDOM*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 414

**Session:** Proteins: Crosslinking - Poster Hall

**Novel techniques for affinity enrichment of crosslinked peptides for studying multi-component protein complex structures by crosslinking combined with mass spectrometry.**

EVGENIY PETROTCHENKO; Christoph Borchers; *UVic-GBC Proteomics Centre, Victoria, CANADA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 415

**Session:** Proteins: Crosslinking - Poster Hall

**Application of Reductive Amination to Protein Crosslinking**

Nagarajan Chandramouli; Joseph P Fernandez; Haiteng Deng; *Proteomics Resource Center, Rockefeller University, New York, NY*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 416

**Session:** Proteins: Crosslinking - Poster Hall

**Identification of a Helicase/Single-Stranded DNA Binding Protein Interaction Site by Mass Spectrometric Analysis**

LAUREN P. BLAIR; Kevin D. Raney; Alan J. Tackett; *UAMS Biochemistry & Molecular Biology, Little Rock, AR*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 417

**Session:** Proteins: Crosslinking - Poster Hall

**Exploring conformational changes of Akt altered by inhibitors using chemical cross-linking and mass spectrometry**

BILL HUANG; Hee-Yong Kim; *NIAAA/NIH, Rockville, MD*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 418

**Session:** Proteins: Crosslinking - Poster Hall

**Identifying interactions between small heat shock proteins and substrate by site directed incorporation of a photoactivatable cross-linker and Mass Spectrometry**

NOMALIE N JAYA; Victor Garcia; Elizabeth Vierling; *University of arizona, Tucson, AZ*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 419

**Session:** Proteins: Crosslinking - Poster Hall

**A Novel Photo-cleavable Protein Interaction Reporter (pcPIR) Cross-linking Strategy to Study Protein-protein Interactions**

Li Yang; Nathan K. Kaiser; Hye In Nam; Haizhen Zhang; Gerhard R. Munske; James E. Bruce; *Washington State Universtij, Pullman, WA*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 420

**Session:** Proteins: Crosslinking - Poster Hall

**Investigating the Detailed Chemistry of Chemical Cross-linking: Reactivities of Different Amino Acids**

Stefanie Mädler; Claudia Bich; David Touboul; Renato Zenobi; *Eth Zurich, Zurich, SWITZERLAND*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 421

**Session:** Proteins: Crosslinking - Poster Hall

**Laser Induced Selective Retrieval of Cross-linked Peptides for Mass Spectrometric Analysis of Protein Complexes**

Funing Yan; Fa-yun Che; Dmitry Rykunov; Edward Nieves; Andras Fiser; Louis M. Weiss; RUTH HOGUE ANGELETTI; *Albert Einstein College of Medicine, Bronx, NY*

**Code:** Monday - MPP

**Time Slot/Poster Number:** 422

**Session:** Proteins: Crosslinking - Poster Hall

**Interactions of the Peroxisome Proliferator-Activated Receptor alpha (PPAR $\alpha$ ) with Ligands Analyzed by Chemical Cross-Linking and Nano-HPLC/MALDI-TOF/TOF-MS and HPLC/ESI-FTICR-MS**

Mathias Mueller<sup>1</sup>; Christian Ihling<sup>1</sup>; Leo J. de Koning<sup>2</sup>; Ronald Aardema<sup>2</sup>; Henk L. Dekker<sup>2</sup>; Yvonne Syha<sup>3</sup>; Manfred Schubert-Zsilavec<sup>3</sup>; Chris G. de Koster<sup>2</sup>; ANDREA SINZ<sup>1</sup>; *Martin Luther University Halle-Wittenberg, Halle, GERMANY*; <sup>2</sup>*Universiteit van Amsterdam, Amsterdam, The Netherlands*; <sup>3</sup>*Johann-Wolfgang-Goethe University Frankfurt, Frankfurt, Germany*

**Code:** Monday - MPPP

**Time Slot/Poster Number:** 423

**Session:** Proteins: Membrane - Poster Hall

**Thermodynamic Analysis of Membrane Bound Receptor-Ligand Interactions**

Patrick D. DeArmond<sup>1</sup>; Michael J. Campa<sup>2</sup>; Edward F. Patz, Jr.<sup>2</sup>; Michael C. Fitzgerald<sup>1,1</sup>; *Duke University, Durham, NC*; <sup>2</sup>*Duke University Medical Center, Durham, NC*

**Code:** Monday - MPPP

**Time Slot/Poster Number:** 434

**Session:** Proteins: Membrane - Poster Hall

**The Mechanism and Target of Aliphatic Azides as Novel Protein Photo-labeling Reagents**

DENNIS SZYMANSKI<sup>1</sup>; Lakshmi pathi Pandarinathan<sup>2</sup>; Alexander Makriyannis<sup>2,1</sup>; *Boston, MA*; <sup>2</sup>*Center for Drug Discovery, Boston, MA*

**Code:** Monday - MPPPP

**Time Slot/Poster Number:** 461

**Session:** Protein Conformation - Poster Hall

**What is the Smallest Protein whose Native Fold can be Preserved in a Mass Spectrometer?**

Jason Kalapothakis; Andrew Stopford; PERDITA BARRAN; *The University of Edinburgh, Edinburgh, UNITED KINGDOM*

**Code:** Monday - MPT

**Time Slot/Poster Number:** 641

**Session:** Bioinformatics I - Poster Hall

**HeXicon: Fully Automated HX-MS Data Analysis with Complete Deuteration Distribution Estimation**

Xinghua Lou<sup>1</sup>; Marc Kirchner<sup>1</sup>; Bernhard Y. Renard<sup>1</sup>; Ullrich Koethe<sup>1</sup>; Bjoern M. Voss<sup>1</sup>; Christian Graf<sup>1</sup>; Judith A. J. Steen<sup>2</sup>; Hanno Steen<sup>2</sup>; Matthias P. Mayer<sup>1</sup>; Fred A. Hamprecht<sup>1,1</sup>; *University of Heidelberg, Heidelberg, GERMANY*; <sup>2</sup>*Harvard Medical School/Children's Hospital Boston, Boston, MA*

# TUESDAY

**Code:** Tuesday - TOB am

**Time Slot/Poster Number:** 08:30 am

**Session:** Structure and Energetics of Metal Ions Reacting with Biomolecules - Korbel Ballroom 1

**The Versatility of Mass Spectrometry Applied to Metal-Biomolecule Interactions**

RICHARD VACHET; *University of Massachusetts, Amherst, MA*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 08:30 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Ionic Cross-linking Reagents and Multistage Tandem Mass Spectrometry for Mapping Protein-Protein Interactions**

Yali Lu; Marina Tanasova; Babak Borhan; GAVIN E. REID; *Michigan State University, East Lansing, MI*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 08:50 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Novel collision-induced dissociative chemical crosslinking reagents and methodology to characterize protein-protein interactions using tandem mass spectrometry**

Erik J. Soderblom; Michael B. Goshe ; *NC State University, Raleigh, NC*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 09:10 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Novel Subunit Specific Protein Footprinting Method Reveals HIV Integrase Contacts with Viral DNA**

Zhuojun Zhao; Christopher McKee; Jacques Kessi; Jocelyn Norris; Nick Shkriabai; Mamuka Kvaratskhelia; *The Ohio State University, Columbus, OH*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 09:30 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Profiling protein-protein interactions in vivo by cross-linking and mass spectrometry**

SAIFUL M. CHOWDHURY<sup>1</sup>; Liang Shi<sup>1</sup>; Xiuxia Du<sup>1</sup>; Uljana M. Mayer-Cumblidge<sup>1</sup>; Nikola Tolic<sup>1</sup>; Yoon Hyunjin<sup>2</sup>; Ronald J. Moore<sup>1</sup>; Norbeck D. Angela<sup>1</sup>; Fred Heffron<sup>2</sup>; Joshua N. Adkins<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific North West National Laboratory, Richland, WA*; <sup>2</sup>*Oregon Health & Science University, Portland, OR*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 09:50 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Identification of Cross-Linked Peptides in Proteomic-Scale Experiments.**

Morten Rasmussen; Salman Tahir; Zhuo Chen; Juri Rappsilber; *Wellcome Trust Centre for Cell Biology, Edinburgh, UNITED KINGDOM*

**Code:** Tuesday - TOG am

**Time Slot/Poster Number:** 10:10 am

**Session:** Biological Applications of Chemical Crosslinking - Rooms 601-607

**Identification of Crosslinked Peptides by an "open-modification" search tool**

PRAGYA SINGH<sup>1</sup>; Scott A. Shaffer<sup>1</sup>; Alexander Scherl<sup>1</sup>; Ted L. Freeman<sup>1</sup>; Carole Holman<sup>1</sup>; Richard A. Pfuetzner<sup>1</sup>; Samuel I. Miller<sup>1</sup>; Patricia Hernandez<sup>2</sup>; Ron D. Appel<sup>2</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Swiss Institute of Bioinformatics, Geneva, Switzerland*

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 2:30 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Resolving protein folding mechanisms with mass spectrometry**

PATRICK WINTRODE; *Case Western Reserve Univ., Cleveland, OH*

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 2:50 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Probing the Conformation and Dynamics of a Monoclonal Antibody by Hydrogen-Deuterium Exchange Mass Spectrometry**

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

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 3:10 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Conformational dynamics of Hsp90 chaperones measured by amide hydrogen exchange mass spectrometry**

Christian Graf; Marta Stankiewicz; Günter Kramer; MATTHIAS P. MAYER; Zentrum für Molekulare Biologie der Universität He, Heidelberg, GERMANY

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 3:30 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Conformational consequences of covalent modification of protein pharmaceuticals under stress-like conditions: ESI MS study of interferon beta**

Cedric Bobst<sup>1</sup>; Rinat R. Abzalimov<sup>1</sup>; Damian Houde<sup>2</sup>; Steven A. Berkowitz<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

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 3:50 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Structural mechanism of HK97 capsid expansion monitored by x-ray crystallography and Hydrogen Deuterium exchange coupled with mass spectrometry**

ILYA GERTSMAN; Jack Johnson; Scripps research institute, la jolla, CA

**Code:** Tuesday - TOE pm

**Time Slot/Poster Number:** 4:10 pm

**Session:** H/D Exchange and Protein Folding - Four Season Ballroom 1-2

**Are the Conformational Dynamics of Enzymes Enhanced During Catalytic Turnover? A Hydrogen/Deuterium Exchange ESI-MS Study**

YU-HONG LIU; Lars Konermann; The University of Western Ontario, London, CANADA

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**Code:** Tuesday - TPC

**Time Slot/Poster Number:** 082

**Session:** ECD/ETD/EDD - Poster Hall

**Electron Transfer Dissociation Facilitates the Measurement of Deuterium-Incorporation into Selectively Labeled Peptides with Single Residue Resolution**

Martin Zehl; Kasper D. Rand; Ole N. Jensen; Thomas J. D. Jørgensen; University of Southern Denmark, Odense, DENMARK

**Code:** Tuesday - TPI

**Time Slot/Poster Number:** 229

**Session:** Noncovalent Interactions I - Poster Hall

**Quantitative Determination of Metal-Protein Dissociation Constants Using Metal-Catalyzed Oxidation Reactions and Mass Spectrometry**

ADAM M GRAICHEN; Richard Vachet; University of Massachusetts, Amherst, MA

**Code:** Tuesday - TPI

**Time Slot/Poster Number:** 232

**Session:** Noncovalent Interactions I - Poster Hall

**SUPREX Analysis of a Misfolded Disease-Related Variant of Alanine:Glyoxylate Aminotransferase**

Erin D. Hopper; Adrienne M.C. Pittman; Chandra Tucker; Michael C. Fitzgerald; Duke University, Durham, NC

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 495

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Limited Proteolysis and Oxidative Surface Mapping for Characterization of the DNA-Binding Domain of Mismatch Repair Protein Pms1 by Mass Spectrometry**

Allison N Schorzman<sup>1</sup>; Jenny M Cutalo<sup>2</sup>; Lars C Pedersen<sup>1</sup>; Thomas A Kunkel<sup>1</sup>; Kenneth B. Tomer<sup>1</sup>; <sup>1</sup>NIEHS, Research Triangle Park, NC; <sup>2</sup>Federal Bureau of Investigation, Quantico, VA

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 496

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Conformational studies of a monoclonal antibody, IgG1, by chemical oxidation: Structural analysis by ultra performance LC-ESI-ToFMS and multivariate data analysis**

LEILA ZAMAN<sup>1</sup>; Fredrik O. Andersson<sup>2</sup>; Yang Yang<sup>2</sup>; Per Edebrink<sup>2</sup>; Sven P. Jacobsson<sup>2</sup>; <sup>1</sup>Stockholm University, Stockholm, SWEDEN; <sup>2</sup>AstraZeneca, Södertälje, Sweden

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 497

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Experimental and Informatic Aspects of Electrochemical Oxidation as a Surface Mapping Probe for Higher Order Protein Structure**

CARLEE MCCLINTOCK; Vilmos Kertesz; Susie Dai; Robert Hettich; *Oak Ridge National Laboratory, Oak Ridge, TN*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 498

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**FPOP Labels Proteins Faster than They Unfold.**

Brian C. Gau<sup>1</sup>; Joshua S. Sharp<sup>2</sup>; Don L. Rempel<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO; <sup>2</sup>University of Georgia, Athens, GA

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 499

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Monitoring Conformational Changes of the Bacillus anthracis Protective Antigen with Differential Oxidative Surface Mapping**

JAMES G. SMEDLEY, III<sup>1</sup>; Joshua S. Sharp<sup>2</sup>; Jeffrey F. Kuhn<sup>3</sup>; Kenneth B. Tomer<sup>1</sup>; <sup>1</sup>NIEHS, Durham, NC; <sup>2</sup>University of Georgia, Athens, GA; <sup>3</sup>Varian Analytical Instrum, Cary, NC

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 500

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Use of oxidation and mass spectrometry to elucidate the function mechanism of a DNA-architecture protein**

Françoise Culard; Corinne Bure; Melanie Spothem; MARTINE CADENE; *CBM du CNRS, ORLEANS cedex 02, FRANCE*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 501

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Probing the Structure of Short-Lived Protein Folding Intermediates by Hydroxyl-Radical-Mediated Oxidative Labeling and ESI-MS**

BRADLEY B. STOCKS; Lars Konermann; *Univ. of Western Ontario, London, ON*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 502

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Substrate Binding Inhibits Chemical Modification of Human Bile Acid CoA:Amino Acid N-acyltransferase (hBAT)**

ERIN M SHONSEY; Stephen Barnes; Matthew B Renfrow; *UAB, Birmingham, AL*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 503

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Structural Characterization of the Calcium Binding Protein Calbindin-D28k**

Carey A. Hobbs<sup>1</sup>; Leesa J. Deterding<sup>2</sup>; Richele J. Thompson<sup>1</sup>; Benjamin G. Bobay<sup>1</sup>; Kenneth Tomer<sup>2</sup>; John Cavanagh<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>NIEHS, Research Triangle Park, NC

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 504

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Protein surface mapping by employing hydroxyl radicals, mass spectrometry and molecular dynamics simulations**

OLGA CHARVATOVA<sup>1</sup>; B. Lachele Foley<sup>1</sup>; Marshall W. Bern<sup>2</sup>; Joshua S. Sharp<sup>1</sup>; Ron Orlando<sup>1</sup>; Robert J. Woods<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Palo Alto Research Center, Palo Alto, CA

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 505

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Surface Mapping of  $\beta$ -2-Microglobulin Oligomers Using Covalent Labeling and Top-down Sequencing**

MARK OLBRIS<sup>1</sup>; Vanessa Leah Mendoza<sup>2</sup>; Richard Vachet<sup>2</sup>; <sup>1</sup>Univ. of Massachusetts, Amherst, MA; <sup>2</sup>University of Massachusetts, Amherst, MA

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 506

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Probing the structure of serpin/protease complexes by structural mass spectrometry method**

XIAOJING ZHENG; Patrick Wintrode; Mark Chance; *case western reserve univ, cleveland, OH*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 507

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Combining structural mass spectrometry and Rosetta: experimental data constrained de novo structure inference**

KEIJI TAKAMOTO<sup>1</sup>; Xiaojing Zheng<sup>1</sup>; Janna Kiselar<sup>1</sup>; Rhiju Das<sup>2</sup>; Robert Vernon<sup>2</sup>; David Baker<sup>2</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>University of Washington, Seattle, WA

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 508

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Pulsed Electron Beam Water Radiolysis: A Novel Method for Sub-Microsecond Hydroxyl Radical Protein Footprinting**

CAROLINE WATSON<sup>1</sup>; Deanna O'Donnell<sup>2</sup>; Ireneusz Janik<sup>2</sup>; Tiandi Zhuang<sup>1</sup>; James H. Prestegard<sup>1</sup>; Joshua S. Sharp<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>University of Notre Dame, Notre Dame, IN

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 509

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Structural Probing of Snap-Frozen Proteins by X-ray radiolysis and Mass Spectrometry: Radiation Damage at Work**

SAYAN GUPTA; Rhijuta D'Mello; Mark R. Chance; *CWRU-Center for Proteomics, Upton, NY*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 510

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Probing native structures of homologous large proteins with differential covalent labeling and mass spectrometry characterization**

SUSIE DAI; Carlee McClintock; Robert Hettich; *Oak Ridge National Laboratory, Oak Ridge, TN*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 511

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**A novel approach to characterizing prion protein structures using chemical labelling, microwave-assisted acid hydrolysis and MALDI-MS.**

JOSEPHINE S.W. TSANG; Adina Bujold; David Wishart; Liang Li; *University of Alberta, Edmonton, Canada*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 512

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Extension of Fast Photochemical Oxidation of Proteins (FPOP) to Mapping Calmodulin and Calmodulin-Peptide Complexes**

Hao Zhang; Michael L. Gross; *Washington University, Saint Louis, MO*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 513

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Synthesis and structural characterization of polyubiquitin conjugates using high resolution mass spectrometry**

Jieun Jung<sup>1</sup>; Marilena Manea<sup>1</sup>; Hans-Peter Wollscheid<sup>2</sup>; Martin Scheffner<sup>2</sup>; Michael Przybylski<sup>1,1</sup>; *Laboratory of Analytical Chemistry, Konstanz, Germany;* <sup>2</sup>*Laboratory of Cellular Biochemistry, Konstanz, Germany*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 514

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Surface Mapping of rmetG-CSF to Determine Oligomerization Induced Difference in Surface Solvent Exposure at Neutral pH and 37 °C**

SHABNAM FARAHMAND; David M. Hambly; Himanshu S. Gadgil; Gerd R. Kleemann; Michael J. Treuheit; *Amgen, Inc., Seattle, WA*

**Code:** Tuesday - TPSS

**Time Slot/Poster Number:** 515

**Session:** Protein Conformation - Oxidative and Covalent Labeling - Poster Hall

**Ubiquitin conformation and dynamics revealed using selective noncovalent adduct protein probing MS and site-directed mutagenesis**

Zhenjiu Liu<sup>1</sup>; Shijun Cheng<sup>1</sup>; Daniel Gallie<sup>1</sup>; Ryan R. Julian<sup>2,1</sup>; *University of California, Riverside, CA;* <sup>2</sup>*University of California, Riverside, Riverside, CA*

# WEDNESDAY

**Code:** Wednesday - WPE

**Time Slot/Poster Number:** 088

**Session:** Ion Activation - Poster Hall

**Identification of Bis-aryl Hydrazone Crosslinked Peptides by Ultraviolet Photodissociation Mass Spectrometry**

MYLES GARDNER; Jennifer Brodbelt; *University of Texas - Austin, Austin, TX*

**Code:** Wednesday - WPEE

**Time Slot/Poster Number:** 112

**Session:** Ion Molecule Reactions I - Poster Hall

**Gas Phase Hydrogen/Deuterium Exchange of Peptides: Effect of Intramolecular Interactions**

YOUNG LEE; Laura Simpson; Elaine M. Marzluff; *Grinnell College, Grinnell, IA*

**Code:** Wednesday - WPEE

**Time Slot/Poster Number:** 115

**Session:** Ion Molecule Reactions I - Poster Hall

**Gas Phase Hydrogen/Deuterium Exchange of Peptides Containing Acidic Sidechains**

Elaine M. Marzluff; Ning-Shiuan Lee; Spring Knapp; *Grinnell College, Grinnell, IA*

**Code:** Wednesday - WPEE

**Time Slot/Poster Number:** 116

**Session:** Ion Molecule Reactions I - Poster Hall

**Gas-Phase H/D exchange of lysine-containing peptides: impact of conformational changes and intramolecular interactions**

BYOUNG JOON KO<sup>1</sup>; Jennifer Brodbelt<sup>2</sup>; <sup>1</sup>*UT-Austin, Austin, TX*; <sup>2</sup>*The University of Texas, Austin, TX*

**Code:** Wednesday - WPL

**Time Slot/Poster Number:** 242

**Session:** Noncovalent Interactions II - Poster Hall

**The Binding Interface of LexA/RecA Investigated by Solution Phase H/D Exchange, Cross-linking and Mass Spectrometry**

BRITTANY R. PERKINS; Guilong Cheng; Kim Giese; Vicki H. Wysocki; John W. Little; *University of Arizona, Tucson, AZ*

**Code:** Wednesday - WPP

**Time Slot/Poster Number:** 334

**Session:** Small Molecule Analysis - Data Processing/Instrumentation - Poster Hall

**Gas Phase Hydrogen Deuterium Exchange of Compounds Introduced by HPLC to a Commercial Mass Spectrometer at mL/min Flow Rates**

David Black; David J. Burinsky; *Glaxosmithkline, Rtp, NC*

**Code:** Wednesday - WPQ

**Time Slot/Poster Number:** 363

**Session:** Immunology - Poster Hall

**Characterization of the Epitope Between IL-13 and 13C5 Using Surface Plasmon Resonance, Covalent Labeling and Epitope Excision Mass Spectrometry**

SHAUN MCLOUGHLIN; Yan Chen; Enrico DiGiammarino; Eric Hebert; Suzanne Scesney; Denise Karaoglu-Hanzatian; Laura Miesbauer; Tanveer Ahmed; Robert Johnson; John Harlan; Chengbin Wu; *Abbott Laboratories, Abbott Park, IL*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 480

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Hydrogen exchange shows that phosphorylation of c-Abl Tyr 89 disrupts downregulatory intramolecular interactions**

SHUGUI CHEN<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 School of Medicine, Pittsburgh, PA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 481

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Mg<sup>2+</sup> concentration-dependence of 70S ribosomal-protein dynamics revealed by H/D exchange and mass spectrometry**

TATSUYA YAMAMOTO; Yoshitsugu Shiro; *RIKEN, Sayo-gun, JAPAN*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 482

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Development of a Structure Based Assay for Characterization of Synthetic Rexinoids by use of Hydrogen Deuterium Exchange Mass Spectrometry**

LeeAnn J. Boerma; Gang Xia; Sebyung Kang; Donald Muccio; Matthew B. Renfrow; *UAB at Birmingham, Birmingham, AL*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 483

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Probing conformational dynamics of PEGylated proteins with hydrogen/deuterium exchange and mass spectrometry**

Rinat R. Abzalimov; IGOR A. KALTASHOV; *University of Massachusetts, Amherst, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 484

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Identification of the Oligomerization Surface of the gp3 Subunit of the Bacteriophage P22 Using Hydrogen Exchange**

LISA M. JONES<sup>1</sup>; Daniel Nemecek<sup>2</sup>; Matthew B. Renfrow<sup>1</sup>; George J. Thomas, Jr.<sup>2</sup>; Peter E. Prevelige, Jr.<sup>1</sup>; *<sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Missouri-Kansas City, Kansas City, Missouri*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 485

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Conformational changes in HIV Nef upon myristoylation as determined by hydrogen exchange mass spectrometry**

Chris R. Morgan<sup>1</sup>; Purushottam Narute<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*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 486

**Session:** Protein Conformation HD Exchange I - Poster Hall

**The effects of mutation and inhibitor binding on Abl kinase conformation by hydrogen deuterium exchange mass spectrometry**

ROXANA E. IACOB<sup>1</sup>; Teodora Pene-Dumitrescu<sup>2</sup>; Nathanael S. Gray<sup>3</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>4</sup>; *<sup>1</sup>Barnett Institute, NEU, Boston, MA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA; <sup>3</sup>Dana-Farber Cancer Institute, Harvard Medical, Boston, MA; <sup>4</sup>Northeastern University, Boston, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 487

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Characterization of the modular organization of p47phox by hydrogen/deuterium exchange**

Julien Marcoux<sup>1</sup>; Petr Man<sup>1</sup>; Corinne Vives<sup>2</sup>; Franck Fieschi<sup>2</sup>; Eric Forest<sup>1</sup>; *<sup>1</sup>LSMP - Institut de Biologie Structurale, Grenoble, France; <sup>2</sup>LPM - Institut de Biologie Structurale, Grenoble, France*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 488

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Conformational Analysis of the HIV-1 viral infectivity factor (Vif) Protein using Hydrogen Exchange Mass Spectrometry**

SEAN R. MARCSISIN<sup>1</sup>; Dana Gabuzda<sup>2</sup>; K.S. Rajendran<sup>2</sup>; Andrew J. Brazier<sup>2</sup>; John Engen<sup>1</sup>; *<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 489

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Local Unfolding of hWT and Three ALS-mutant SOD1 Apoproteins at Physiological Temperatures Monitored by Hydrogen/Deuterium Exchange Mass Spectrometry.**

ARMANDO DURAZO<sup>1</sup>; Bryan F. Shaw<sup>4</sup>; Madhuri Chattopadhyay<sup>1</sup>; Julian Whitelegge<sup>2</sup>; Kym Faulk<sup>3</sup>; Joan S. Valentine<sup>1</sup>; *<sup>1</sup>UCLA Chemistry, Los Angeles, CA; <sup>2</sup>University of California La, Los Angeles, CA; <sup>3</sup>Ucla, Los Angeles, CA; <sup>4</sup>Harvard University, Cambridge, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 490

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Structural Investigation of C-Kit Tyrosine Kinase by Hydrogen/Deuterium Exchange Coupled with FT-ICR Mass Spectrometry**

HUIMIN ZHANG<sup>1</sup>; Xiu Yu<sup>2</sup>; Michael Greig<sup>2</sup>; Wade Diehl<sup>2</sup>; Ketan Gajiwala<sup>2</sup>; You-Ai He<sup>2</sup>; Elizabeth Lunney<sup>2</sup>; Alan G. Marshall<sup>1</sup>; Mark R. Emmett<sup>1</sup>; *<sup>1</sup>Nat'l High Magnetic Field Lab, Florida State Univ., Tallahassee, FL; <sup>2</sup>Pfizer Global, R&D- La Jolla, San Diego, CA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 491

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Probing an Integrin I Domain Structure With Enhanced H/D Exchange Mass Spectrometry (DXMS) and Differential Scanning Calorimetry (DSC)**

Sheng Li<sup>2</sup>; Tong Liu<sup>2</sup>; Paul H. Weinreb<sup>1</sup>; Samantha Phan<sup>1</sup>; Stephen Demarest<sup>1</sup>; Alexander Buko<sup>1</sup>; R. Blake Pepinsky<sup>1</sup>; Virgil Woods, Jr.<sup>2</sup>; Sharon Gao<sup>1,1</sup>; *Biogenidec, Inc., San Diego, CA 92121*;

<sup>2</sup>*University of California, La Jolla, CA 92093*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 492

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Semi-automated Hydrogen Deuterium Exchange (HDX) for the analysis of dynamics and structure of viral poly(A) polymerase**

Marek Daniel Koter; Paul David Gershon; *University of California,, Irvine, CA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 493

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Assembly of Matrix Protein VP40 of Ebola Virus by Hydrogen-Deuterium Exchange Mass Spectrometry**

LESLIE SILVA<sup>1</sup>; M. Javad Aman<sup>2</sup>; David Schriemer<sup>1,1</sup>; *University of Calgary, Calgary, CANADA*; <sup>2</sup>*U.S. Medical Research Inst. of Infectious Disease, Fredrick, MD*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 494

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Towards the Identification of the CRABP II and RAR Regions Involved in RA Transfer Using HDX and Chemical Crosslinking**

VIRGINIE SJOELUND; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 495

**Session:** Protein Conformation HD Exchange I - Poster Hall

**How do infectious bacteria protect themselves? H/D exchange mass spectrometry probes the answer.**

Justin B. Sperry; Craig L. Smith; Michael G. Caparon; Scott J. Hultgren; Thomas E. Ellenberger; Michael L. Gross; *Washington University in St. Louis, St. Louis, MO*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 496

**Session:** Protein Conformation HD Exchange I - Poster Hall

**The Iron Binding Mechanism of Human Transferrin Examined by Hydrogen Deuterium Exchange Mass Spectrometry**

CEDRIC BOBST<sup>1</sup>; Igor A. Kaltashov<sup>2,1</sup>; *University of Massachusetts, Amherst, Amherst, MA*; <sup>2</sup>*University of Massachuset, Amherst, MA*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 497

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Factors Affecting Hydrogen-deuterium Exchange at the MHC-peptide Binding Interface**

SACHIN PATIL; Hermann von Grafenstein; *University of Toledo, Toledo, OH*

**Code:** Wednesday - WPTTT

**Time Slot/Poster Number:** 498

**Session:** Protein Conformation HD Exchange I - Poster Hall

**Using HX-ESI-MS to investigate the amyloidogenic protein beta-2-microglobulin in its monomeric state and when bound within the major histocompatibility complex.**

John P Hodkinson<sup>1</sup>; Thomas R Jahn<sup>2</sup>; Sheena E Radford<sup>1</sup>; Alison E Ashcroft<sup>1,1</sup>; *University of Leeds, Leeds, UK*; <sup>2</sup>*University of Cambridge, Cambridge, UK*

# THURSDAY

**Code:** Thursday - ThOD am

**Time Slot/Poster Number:** 08:50 am

**Session:** Structural Biology and Biophysics of Nucleic Acids - Korbel Ballroom 4

**DNA-MEDIATED REF1 CONFORMATIONAL CHANGES: POSSIBLE MECHANISM FOR PROTEIN RECRUITMENT IN BASE EXCISION REPAIR (BER) PATHWAY**

Eizadora T. Yu<sup>1</sup>; Sara P. Gaucher<sup>2</sup>; Kenneth Sale<sup>1</sup>; Masood Z. Hadi<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Livermore, CA; <sup>2</sup>Amyris Biotechnologies, Emeryville, CA

**Code:** Thursday - ThOD am

**Time Slot/Poster Number:** 09:10 am

**Session:** Structural Biology and Biophysics of Nucleic Acids - Korbel Ballroom 4

**Modeling stable conformers of the 5' non-coding region of HIV-1 genome using sparse constraints provided by MS-based strategies**

Jiarong Xia; Dong Yang; Alberto Berton; Daniele Fabris; *Univeristy of Maryland Baltimore County, Baltimore , MD*

**Code:** Thursday - ThOE pm

**Time Slot/Poster Number:** 3:50 pm

**Session:** Ionization and Characterization of Macromolecules and Complexes - Four Seasons Ballroom 1-2

**Combined Covalent Labeling Methods for Studying  $\beta$ 2m Oligomer Assembly by MS**

Vanessa Leah Mendoza; Srikanth Rapole; Mark R. Olbris; Richard W. Vachet; *University of Massachusetts, Amherst, MA*

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**Code:** Thursday - ThPB

**Time Slot/Poster Number:** 059

**Session:** Ion Mobility Applications - Poster Hall

**Detection of Oligonucleotide Gas-Phase Conformers by Combined H/D Exchange and Ion Mobility**

Dorothee Balbeur<sup>1</sup>; Joëlle Widart<sup>1</sup>; Bernard Leyh<sup>2</sup>; Laetitia Cravello<sup>3</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>LSM at the ULg, Liège, BELGIUM; <sup>2</sup>Molecular Dynamics Laboratory, Liège, Belgium; <sup>3</sup>Waters Corporation, Manchester, United Kingdom

**Code:** Thursday - ThPC

**Time Slot/Poster Number:** 072

**Session:** Instrumentation: Ion Sources, General - Poster Hall

**Determination of Rapid H/D Exchange Number of Solid Peptides and Proteins by Electrospray-Assisted Laser Desorption Ionization (ELDI) Mass Spectrometry**

Li-Hua Lo<sup>1</sup>; Jinyueh Jeng<sup>2</sup>; Yi-Tzu Cho<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen Univ., Kaohsiung, TAIWAN; <sup>2</sup>Chia Nan University of Pharmacy & Science, Tainan, Taiwan

**Code:** Thursday - ThPDD

**Time Slot/Poster Number:** 108

**Session:** Ion Structures/Energetics II - Poster Hall

**Computational Modeling of the H/D Exchange Behavior of Asparagine and Its O-Methyl Ester**

Brooklynd Saar<sup>1</sup>; Elise Dennis<sup>1</sup>; Brittany R. Perkins<sup>2</sup>; John Poutsma<sup>1</sup>; Vicki H. Wysocki<sup>2</sup>; <sup>1</sup>College of William & Mary, Williamsburg, VA; <sup>2</sup>University of Arizona, Tucson, AZ

**Code:** Thursday - ThPDD

**Time Slot/Poster Number:** 112

**Session:** Ion Structures/Energetics II - Poster Hall

**Gas-phase H/D exchange of deprotonated glycine oligomers (Gly)<sub>n</sub> (n=1-6)**

Zhixin Tian; Steven R. Kass; *Department of Chemistry, University of Minnesota, Minneapolis, MN*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 491

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Hydrogen/Deuterium Exchange: Electrospray Ionization Mass Spectrometry for Probing Structural Changes in Proteins Upon Microwave Irradiation**

Urooj A. Mirza; Birendra N. Pramanik; Ajay K. Bose; *Schering Plough Institute, Kenilworth, NJ*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 492  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**HD Desktop: A web based software application for rapid analysis and visualization of hydrogen exchange mass spectra**  
BRUCE D. PASCAL; Michael J. Chalmers; Scott A. Busby; Patrick R. Griffin; *The Scripps Research Institute, Jupiter, FL*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 493  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Recent advances in UPLC for hydrogen exchange mass spectrometry: high-speed & high-resolution separations at zero degrees celsius**  
Thomas E. Wales<sup>1</sup>; Keith Fadgen<sup>2</sup>; Geoff Gerhardt<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 494  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Extension of a SUPREX with Protease Digestion Protocol to Multimeric Proteins**  
YING XU<sup>1</sup>; Michael C. Fitzgerald<sup>2</sup>; <sup>1</sup>*Department of Chemistry, Duke University, Durham, NC*; <sup>2</sup>*Duke University, Durham, NC*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 495  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Control of back exchange and experimental reproducibility for the detection of protein conformational changes by hydrogen exchange mass spectrometry**  
WILLIAM I BURKITT; Gavin O'Connor; *LGC, London, UNITED KINGDOM*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 496  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Mass Spectrometric Method to Determine pKa Values of Individual Histidine Residues in Proteins**  
MASARU MIYAGI<sup>1</sup>; Takashi Nakazawa<sup>2</sup>; <sup>1</sup>*Case Western Reserve Univers, Cleveland, OH*; <sup>2</sup>*Nara Women's University, Nara, JAPAN*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 497  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Reduced Labeling and its Benefits for HDX-MS Protocols**  
Andrew J. Percy; Gordon W. Slysz; David C. Schriemer; *University of Calgary, Calgary, CANADA*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 498  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Conformer Structures of Gaseous Protein Ions from Deuteration Effects on Infrared Photodissociation Spectra**  
XIANGLEI KONG<sup>1</sup>; Giuseppe Infusini<sup>2</sup>; Cheng Lin<sup>2</sup>; Honghai Jiang<sup>1</sup>; Kathrin Breuker<sup>3</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>*Cornell University, Ithaca, NY*; <sup>2</sup>*Boston U School of Medicine, Boston, MA*; <sup>3</sup>*University of Innsbruck, Innsbruck, AUSTRIA*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 499  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Gas Phase H/D Exchange of Hemoglobin Monomers, Dimers and Tetramers**  
P. John Wright; Donald J. Douglas; *University of British Columbia, Vancouver, BC*

**Code:** Thursday - ThPTTT  
**Time Slot/Poster Number:** 500  
**Session:** Protein Conformation H/D Exchange II - Poster Hall  
**Comparing peloruside and laulimalide induced microtubule stabilization using HDX and data-directed ligand docking**  
Torin Huzil<sup>2</sup>; Jack Tuszyński<sup>2</sup>; Melissa Bennett<sup>1</sup>; David Schriemer<sup>1</sup>; <sup>1</sup>*University of Calgary, Calgary, Canada*; <sup>2</sup>*University of Alberta, Edmonton, Canada*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 501

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Effects of RPLC separation conditions on back-exchange in solution-phase hydrogen/deuterium exchange mass spectrometry.**

George M. Bou-Assaf<sup>1</sup>; Mark R. Emmett<sup>2</sup>; Alan G. Marshall<sup>2,1</sup>; *Florida State University, Tallahassee, FL;*<sup>2</sup>*Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 502

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Can ETD accurately measure the H/D exchange of individual residues in proteins? – a study of the amyloidogenic protein  $\beta$ -2-microglobulin**

KASPER D. RAND; Martin Zehl; Ole N. Jensen; Thomas J.D. Jørgensen; *University of Southern Denmark, Odense, DENMARK*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 503

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Software for the semi-automated analysis of MALDI-TOF-generated Hydrogen Deuterium Exchange (HDX) data**

Pornpat Nikamanon; Elroy Pun; Wayne Chou; Marek Daniel Koter; Paul David Gershon; *University of California, Irvine, CA*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 504

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**HYDRA: a flexible software package for 'one-click' HDX-MS data analysis**

Gordon W. Slysz; CJ Baker; Benjamin M. Bozsa; Anthony Dang; David C. Schriemer; *University of Calgary, Calgary, CANADA*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 505

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Measurement of protein structure and folding differences associated with systematic mutations of the protein staphylococcal nuclease using HX-HPLC-ESI-MS.**

Rohana Liyanage; Nagarjuna Devarapalli; Latisha M. Puckett; Jennifer Gidden; Wesely E. Stites; Jackson O. Lay, Jr.; *University of Arkansas, Department of Chemistry, Fayetteville, AR, 72701*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 506

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Dual Protease On-line Digestion for High Density Protein Mapping of Large Proteins in Hydrogen/Deuterium Exchange Mass Spectrometry**

SUSAN L. CHEN<sup>1</sup>; Virgil Woods, Jr.<sup>2</sup>; Roland S. Annan<sup>1,1</sup>; *GlaxoSmithKline, King of Prussia, PA;*<sup>2</sup>*University of California, La Jolla, CA*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 507

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Implementing HDX-MS data in directed docking applications: rationalizing amplitude with MD simulations.**

Evan Kelly; Melissa Bennett; Gordon Slysz; Andrew Percy; Hiroaki Ishida; Hans Vogel; DAVID SCHRIEMER; *University of Calgary, Calgary, CANADA*

**Code:** Thursday - ThPTTT

**Time Slot/Poster Number:** 508

**Session:** Protein Conformation H/D Exchange II - Poster Hall

**Using IM-MS and HDX-MS to study native protein conformations**

HANNAH FLORANCE<sup>1</sup>; Peter Faull<sup>1</sup>; Jason Kalapothakis<sup>1</sup>; Bryan J. McCullough<sup>2</sup>; Ted R. Hupp<sup>1</sup>; Perdita Barran<sup>1,1</sup>; *The University of Edinburgh, Edinburgh, UNITED KINGDOM;*<sup>2</sup>*The University of Manchester, Manchester, United Kingdom*

**Code:** Thursday - ThPU

**Time Slot/Poster Number:** 510

**Session:** Proteins - General, Methods - Poster Hall

**The Specificity of Pepsin for Proteolytic Digestion and MS Applications**

MELISSA H. PALASHOFF<sup>1</sup>; Martha Stapels<sup>2</sup>; Keith Fadgen<sup>2</sup>; John R. Engen<sup>1,1</sup>; *Northeastern University, Brighton, MA;*<sup>2</sup>*Waters Corporation, Milford, MA*

**Code:** Thursday - ThPV

**Time Slot/Poster Number:** 532

**Session:** Proteomics: Biomarker Assays II - Poster Hall

**Antibody Characterization for the Development of a Standardized Immunoassay for Human Cardiac Troponin I**

Mark S. Lowenthal; Nathan G. Dodder; Hua-Jun He; Kenneth D. Cole; David M. Bunk; Lili Wang; *National Institute of Standards and Technology, Gaithersburg, MD*

**Code:** Thursday - ThPX

**Time Slot/Poster Number:** 640

**Session:** Bioinformatics IV - Poster Hall

**Computational Methods for Probing Bio-molecular Structures using Protein Footprinting**

Parminder Kaur; J. K. Amisha Kamal; Mark R. Chance; *Center for Proteomics, Case Western Reserve Univ., Cleveland, OH*