

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

ASMS 2007
Indianapolis, Indiana

<u>DAY</u>	<u>Orals</u>	<u>Posters</u>	<u>Total</u>	<u>2006 Total</u>
Monday	15	35	50	15
Tuesday	7	40	47	32
Wednesday	13	43	56	16
Thursday	7	13	19	55
TOTAL	42	131	173	118

List is as all-inclusive as possible. Does not include iTRAQ, ICAT, 16O/18O, SILAC, HysTag, SeMet, or other quantitative labeling strategies, natural modifications

MONDAY

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 09:15
Electrospray Ionization Mass Spectrometry of the Interaction of Oligonucleotides with Metals, Small Molecules and Drugs

Janna Anichina; Diethard K. Bohme
York University, Department of Chemistry, Toronto, CANADA

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 09:35
Top-down Mass Spectrometry of Noncovalent Protein Complexes for Determining Ligand Binding Sites

Sheng Yin¹; Vlad Zabrouskov²; Joseph A. Loo¹
¹*UCLA, Los Angeles, CA*; ²*Thermo Scientific, San Jose, CA*

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 09:55
Zinc uptake and release by metallothioneins and their regulators from bacteria and plants

Claudia A Blindauer; Oksana Leszczyszyn; Joanne Palmer; Kowald Gregory
University of Warwick, Coventry, UNITED KINGDOM

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 10:15
The Role of Alkali Metals in Helix Stabilization

Janel R McLean; John A. McLean; David H. Russell
Texas A & M University, College Station, TX

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 10:35
A molecular basis for enhancing phytoremediating plants through genetic modification – an atomic and molecular MS study

Joseph A. Caruso¹; Kevin Kubachka¹; Juris Meija¹; Danika LeDuc²
¹*University of Cincinnati, Cincinnati, OH*; ²*California State Univ. East Bay, Hayward, CA*

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** MOG am **Time Slot/Poster Number:** 10:55
Proteomic Characterization of Spinal Cord Lipid Raft Proteins in ALS

Jianjun Zhai; Anna-Lena Strom; Zhenyu Huang; Renee Kilty; Priya Venkatakrisnan; Eric Smart; Haining Zhu
University of Kentucky, Lexington, KY

Session: Invited Presentation **Code:** MOB pm **Time Slot/Poster Number:** 03:30

Mass Spectrometric Determination of Factors Governing the Formaldehyde Cross-Linking Reaction and their Relevance for Protein Interaction Studies in Live Cells

Judy Toews; Peter Schubert; Brent Sutherland; Juergen Kast
University of British Columbia, Vancouver, CANADA

Session: Characterizing Cross-Linked Proteins with MS **Code:** MOB pm **Time Slot/Poster Number:** 03:50
Novel isotopically-coded crosslinkers for structural proteomics.

Evgeniy Petrotchenko; Christoph Borchers
University of Victoria Genome BC Proteomics Centre, Victoria, Canada

Session: Characterizing Cross-Linked Proteins with MS **Code:** MOB pm **Time Slot/Poster Number:** 04:10
Crosslinked Peptide Data Obtained by Ion Mobility used to Sort Correct/Incorrect in silico Protein Conformation Predictions

David R. Goodlett¹; Lars Malmstroem¹; Chris Hughes²; Pragma Singh¹; Chunsheng Zhao¹; Alex Scherl¹; Jie Liu³; Scott Shaffer¹; James Langridge²
¹*University of Washington, Seattle, WA*; ²*Waters Corporation, Manchester, UK*; ³*Shenzhen Nanshan Center, Shenshen, CHINA*

Session: Characterizing Cross-Linked Proteins with MS **Code:** MOB pm **Time Slot/Poster Number:** 04:30
Combined LC-ESI-MS/MS and LC-MALDI-MS/MS analysis reveals an unusual protein-RNA contact in human [U1snRNP-snurportin1] particles

Eva KÄ¼hn-HÄ¼lsken¹; Christof Lenz²; Florian Richter¹; Monika Raabe¹; Uwe PleÄmann¹; Henning Urlaub¹
¹*Max-Planck-Institute for Biophysical Chemistry, GÄ¼ttingen, Germany*; ²*Applied Biosystems Europe, Darmstadt, Germany*

Session: Characterizing Cross-Linked Proteins with MS **Code:** MOB pm **Time Slot/Poster Number:** 04:50

Identification of cross-linked peptides from complex samples with full proteome protein databases

Oliver Rinner¹; Jan Seebacher²; Martin Beck¹; Alexander Schmidt¹; Thomas Walzthoeni¹; Lukas Mueller¹; Markus Mueller¹; Ruedi Aebersold¹

¹Swiss Federal Institute of Technology, Zurich, SWITZERLAND; ²Harvard Medical School, Boston, MA

Session: Characterizing Cross-Linked Proteins with MS **Code:** MOB pm **Time Slot/Poster Number:** 05:10

Identification of outer membrane protein OmcA-MtrC interactions in Shewanella oneidensis MR-1 cell in vivo using novel cross-linker and mass spectrometry

Haizhen Zhang¹; Xiaoting Tang¹; Natalia Zakharova¹; Gerhard R. Munske¹; Megan A. Wolff¹; Liang Shi²; James K. Fredrickson²; Nikola Tolic²; Gordon A. Anderson²; James E. Bruce¹

¹Washington State University, Pullman, WA; ²Pacific Northwest National Laboratory, Richland, WA

Session: Non-covalent Interactions **Code:** MOE pm **Time Slot/Poster Number:** 03:50

The Role of Phosphorylated Residues in Peptide-Peptide Noncovalent Complexes

SHELLEY N JACKSON; Amina S Woods

NIDA-IRP, NIH, Baltimore, MD

Session: Non-covalent Interactions **Code:** MOE pm **Time Slot/Poster Number:** 04:30

Characterisation of noncovalently bound protein-RNA complexes and their role in virus capsid assembly mechanisms using ESI-MS

Alison E. Ashcroft; Gabriela Basnak; Ottar Rolfsson; Simona Francese; Gary S. Thompson; Nicola J. Stonehouse; Peter G. Stockley

University of Leeds, Leeds, , UNITED KINGDOM

Session: Non-covalent Interactions **Code:** MOE pm **Time Slot/Poster Number:** 04:50

Insights into the Folding and Subunit Interactions of Hemoglobin by ESI-MS

BRIAN L. BOYS; Lars Konermann

University of Western Ontario, Ontario, CANADA

Session: Non-Covalent Interactions **Code:** MPU **Time Slot/Poster Number:** 337

Epitope mapping on bovine prion protein using chemical cross-linking and mass spectrometry

Tatiana Pimenova¹; Alexis Nazabal¹; Bernd Roschitzki²; Jan Seebacher³; Oliver Rinner⁴; Renato Zenobi¹

¹ETH Zurich, Zurich, Switzerland; ²Functional Genomics Center Zurich, Zurich, Switzerland; ³University of Washington, Seattle, WA; ⁴Institute for Molecular Systems Biology, ETHZ, Zurich, Switzerland

Session: Toxicology **Code:** MPV **Time Slot/Poster Number:** 347

Isotope Labeling and Mass Spectrometry for Identifying Formaldehyde-induced Histone Modifications and DNA-protein Crosslinks

Kun Lu; Gunnar Boysen; Lina Gao; Leonard B Collins; James A Swenberg

University of North Carolina at Chapel Hill, Chapel Hill, NC

Session: Toxicology **Code:** MPV **Time Slot/Poster Number:** 357

Simultaneous Analysis of Three Forms of Glyoxal-Induced DNA Crosslinks by nanoLC-Nanospray Ionization/Tandem Mass Spectrometry

Yu-Chin Chen; Hauh-Jyun Candy Chen

National Chung Cheng University, Ming-Hsiung, TAIWAN

Session: Peptides: General **Code:** MPX **Time Slot/Poster Number:** 381

Improved Detection of Proteolytic Peptides with and without Chemical Crosslinks by Quadrupole Fractionation Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

Bo Wang; Kristina HÅkansson

University of Michigan, Ann Arbor, MI

Session: Proteins: Modified **Code:** MPZ3 **Time Slot/Poster Number:** 447

The site of modification and mechanism of inactivation of glyceraldehyde-3-phosphate dehydrogenase upon nitration

Vikram Palamalai¹; Masaru Miyagi²

¹University of North Dakota, Grand Forks, ND; ²Case Western Reserve University, Cleveland, OH

Session: Proteins: Modified **Code:** MPZ3 **Time Slot/Poster Number:** 451

Nitration of Tyrosine Residues within eNOS Protein Utilizing Tetranitromethane, with Tryptic Digest and LTQ Mass Spectrometer

Mike Zickus¹

¹Northern Illinois University, DeKalb, IL; ²Medical College of Georgia, Augusta, Georgia

Session: MS of Oxidized Proteins **Code:** MPZ3 **Time Slot/Poster Number:** 457

Covalent Modification of Proteins by Lipid Peroxidation Products: Characterization by Electrospray Ionization and Ion Trap / FT-ICR Mass Spectrometry

Navin Rauniyar; Katalin Prokai-Tatrai; Stanley M. Stevens; Laszlo Prokai

University of North Texas Health Science Center, Fort Worth, TX

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 474

Conformational studies of phosphorylated motif in α -casein using hydrogen exchange mass spectrometry

Shao-Ching Hung; Demetrius R. Dielman; Krishna Kuppannan; Vickie L. Langer; Anton S. Karnoup; Scott A. Young

The Dow Chemical Company, Midland, MI

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 475

Detection and Characterization of AL Light Chain Proteins from Fibrils

Zhenning Hong; Roger ThÃ©berge; Yan Jiang; Amareth Lim; Tatiana Prokaeva; Lawreen H. Connors; Martha Skinner; Catherine E. Costello

Boston University, Boston, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 476

Direct Comparison of Structures of Wild Type- and Mutant Cu/Zn-Superoxide Dismutase by H/D Exchange Mass Spectrometry

Qi Wang¹; Ashutosh Tiwari²; Lawrence J. Hayward²; Jeffrey N. Agar¹

¹Brandeis University, Waltham, MA; ²University of Massachusetts Medical School, Worcester, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 477

Structural examination of the ClpAP protease complex via synchrotron radiolysis and mass spectrometry

Jen Bohon¹; Laura Jennings²; Stuart Licht²; Mark Chance¹

¹Case Western Reserve University, Upton, NY; ²Massachusetts Institute of Technology, Cambridge, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 478

Fluorescence Measurements of a Single Unsolvated Biomolecule: Conformation Fluctuations

Joel H. Parks; Denis Duft; Xiangguo Shi

Rowland Institute at Harvard, Cambridge, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 479

Probing of the Binding Properties of Acetobacter Aceti Citrate Synthase Using PLIMSTEX and Local H/D Exchange

Sandra Kerfoot; Don L. Rempel; T. Joseph Kappock; Michael L. Gross

Washington University, St. Louis, MO

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 480

Comparing the Conformational Dynamics of Enzymes and Non-Enzymatic Proteins by Hydrogen-Deuterium Exchange and ESI-MS

Yuhong Liu; Lars Konermann

University of Western Ontario, London, CANADA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 481

Two non-covalently bound antagonists on the human RXR α LBD protein studied by hydrogen/deuterium exchange and mass spectrometry

Xuguang Yan; David Broderick; Jeff Morre; Michael Schimerlik; Max Deinzer

Oregon State University, Corvallis, OR

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 482

Mass Spectral Analysis of β 2-Microglobulin Oligomers

Mark Olbris; Kwasi Antwi; R. Srikanth; Richard W. Vachet

University of Massachusetts, Amherst, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 483

Gas-phase Conformations of Protonated Serine Octamers, Peptides, and Proteins Using Infrared Photodissociation Spectroscopy with FTMS

Xianglei Kong¹; Giuseppe Infusini²; Cheng Lin²; Honghai Jiang¹; Kathrin Breuker³; Fred. W. McLafferty¹

¹Cornell University, Ithaca, NY; ²Boston University School of Medicine, Boston, MA; ³University of Innsbruck, Innsbruck, Austria

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 484

Gas Phase Conformations of Protein Ions Formed from Two Different Solution Conformations

Jianmin Zhang; D. J. Douglas

University of British Columbia, Vancouver, CANADA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 485

Protein Conformational Changes Monitored by Gamma Ray-induced Hydroxyl Radical Labeling and ESI-MS

Xin Tong; Lars Konermann

University of Western Ontario, London, CANADA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 486

Extending PLIMSTEX by using MALDI/MS

A T MANOHARI Silva; M. L. Gross

Washington University in St. Louis, Mass Spectromet, St. Louis, MO

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 487

Allosteric Activation of BirA Protein Studied by Hydrogen/Deuterium Exchange Mass Spectrometry

Olli Laine; Emily D Streaker; Catherine Fenselau; Dorothy Beckett

University of Maryland, College Park, MD

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 488

Conformational Changes in Opioid-Related Peptides Induced by Membrane-Mimetic Systems as Studied Using Hydrogen/Deuterium Exchange.

Deepa Kunapuram; Chhabil Dass

The University of Memphis, Memphis, TN

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 489

Hydrogen exchange shows that phosphorylation causes changes in intramolecular interactions

Shugui Chen¹; Thomas E. Smithgall²; John R. Engen¹

¹Northeastern University, Boston, MA; ²University of Pittsburgh School of Medicine, Pittsburgh, PA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 490

Modulation of transferrin conformation by metal binding studied by hydrogen exchange and mass spectrometry

Mingxuan Zhang¹; Anne B. Mason²; Igor A. Kaltashov¹

¹University of Massachusetts, Amherst, MA; ²University of Vermont, Burlington, VT

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 491

Identification of the Inter-subunit Interactions Driving Maturation of HIV-1 Capsids using Mass Spectrometry based Hydrogen/Deuterium Exchange

Sebyung Kang; Matthew B. Renfrow; Peter E. Prevelige

University of Alabama at Birmingham, Birmingham, AL

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 492

Hydrogen deuterium exchange mass spectrometry to study the assembly mechanisms of Ebola virus matrix protein VP40

Leslie Silva¹; Michael Vanzile²; M. Javad Aman²; David C. Schriemer¹

¹University of Calgary, Calgary, CANADA; ²US Army Medical Res. Inst. Infectious Disease, Frederick, MD

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 493

Use of multiple proteases to improve resolution and accuracy in hydrogen/deuterium exchange monitored by FT-ICR mass spectrometry

Huimin Zhang¹; Mark R. Emmett¹; SaÅija KazaziÅ†²; Alan G. Marshall¹

¹Florida State University, Tallahassee, FL; ²RuÅ'er BoÅ;koviÅ† Institute, Zagreb, Croatia

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 494

Analysis of SH3 Domain Interactions with HIV Nef Derived from Long-term Non-progressing HIV+ Patients

Thomas E. Wales¹; Lori Emert-Sedlak²; Ronald P. Tribble²; Thomas E. Smithgall²; John R. Engen¹

¹Northeastern University, Boston, MA; ²University of Pittsburgh School of Medicine, Pittsburgh, PA

Session: Non-Covalent Interactions **Code:** MPZ5 **Time Slot/Poster Number:** 495

Mapping the interaction between phosphorylated human growth hormoneâ€ growth hormone receptor using hydrogen/deuterium exchange mass spectrometry

Hari Kosanam¹; Francesco Giorgianni²; Chabbil Dass¹

¹The University of Memphis, Memphis, TN; ²University of Tennessee Health Science Center, Memphis, TN

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 496

Structural characterization of Factor Xa dimers in solution by differential surface modification and mass spectrometry

ROXANA E. IACOB¹; Rima Chattopadhyay²; Shalmali Sen²; Barry R. Lentz²; Kenneth B. Tomer¹

¹Laboratory of Structural Biology, NIEHS, RTP, North Carolina; ²Department of Biochemistry and Biophysics, UNC, Chapel Hill, North Carolina

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 497

Improved Protein Surface Mapping Using Amino Acid Specific Covalent Modifications Combined with Mass Spectrometry

Vanessa Mendoza; Richard W. Vachet

University of Massachusetts, Amherst, MA

Session: Protein Conformation **Code:** MPZ5 **Time Slot/Poster Number:** 498

Interaction of the Cellular Retinoic Acid Binding Protein with the Retinoic Acid Receptor: A Mass Spectrometric Study

Virginie Sjoelund; Igor A. Kaltashov

University of Massachusetts, Amherst, MA

Session: Proteomics: Biomarkers **Code:** MPZ6 **Time Slot/Poster Number:** 512

Analysis of covalent adducts of cytochrome C arising from nitration and oxygen radical oxidation

Jennifer R. Seal; John S. Wishnok; Steven R. Tannenbaum

Massachusetts Institute of Technology, Cambridge, MA

Session: What Does MS Tell us about Protein-Protein Interac **Code:** MPZ8 **Time Slot/Poster Number:** 550

A QTAX-based Tag-team Method to Characterize Protein Interaction Networks

Cortnie Guerrero; Jeff Jones; Yingying Yang; Peter Kaiser; Lan Huang

UC Irvine, Santa Ana, CA

Session: Proteomics: New and Improved Methods **Code:** MPZ8 **Time Slot/Poster Number:** 560

Identifying protein-protein interactions with LC-MALDI/TOF/TOF and cross-linking strategy

Xiaoting Tang¹; Haizhen Zhang¹; Gerhard R. Munske¹; Natalia L. Zakharova¹; Nikola Tollic²; Gordon A. Anderson²; James E. Bruce¹

¹Washington State University, Pullman, WA; ²Pacific Northwest National Laboratory, Richland, WA

TUESDAY

Session: IMS Applications **Code:** TOD am **Time Slot/Poster Number:** 08:15

Use of a travelling wave-based ion mobility mass spectrometry approach to resolve proteins of varying conformation

James H Scrivens¹; Konstantinos Thalassinos¹; Gillian Hilton¹; Susan E Slade¹; Teresa J T Pinheiro¹; Robert H Bateman²; Michael T Bowers³

¹Univ of Warwick, Coventry, UNITED KINGDOM; ²Waters, Manchester, UK; ³UCSB, Santa Barbara, CA

Session: Non-covalent Interactions **Code:** TOD am **Time Slot/Poster Number:** 08:35

Use of Ion Mobility and High Mass Analysis for the Determination of Protein-Protein Interaction and Topology.

Iain D G Campuzano¹; James Langridge¹; Armann Andaya²; Matthew Schenauer²; Julie Leary²

¹Waters Corporation, Manchester, United Kingdom; ²Genome Centre UC Davis, Davis, CA

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TOD am **Time Slot/Poster Number:** 08:55

Interactions between viral accessory proteins and Src-family kinases measured by H/D exchange mass spectrometry

John R. Engen¹; Thomas E. Wales¹; David D. Weis²; Lori Emert-Sedlak³; Thomas E. Smithgall³

¹Northeastern University, Boston, MA; ²University of New Mexico, Albuquerque, NM; ³University of Pittsburgh, Pittsburgh, PA

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TOD am **Time Slot/Poster Number:** 09:15

Comparing SID and CID of Noncovalent Protein-Protein Complexes in a Modified QTOF Mass Spectrometer

Richard L. Beardsley; Christopher M. Jones; Asiri S. Galhena; Vicki H. Wysocki

University of Arizona, Tucson, AZ

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TOD am **Time Slot/Poster Number:** 09:35

Virus assembly studied by macromolecular (tandem) mass spectrometry and ion mobility

Kristina Lorenzen; Charlotte Uetrecht; Cees Versluis; Albert J.R. Heck

Utrecht University, CA Utrecht, NETHERLANDS

Session: IMS Applications **Code:** TOD am **Time Slot/Poster Number:** 09:55

Protein conformational flexibility and structural change upon binding of ligands and proteins studied by ion mobility Q-TOF MS

Stephen J. Watt¹; Iain Campuzano²; Frank Sobott¹

¹Structural Genomics Consortium, Oxford, UNITED KINGDOM; ²Waters Corporation, Manchester, UK

Session: Ion Trap Applications **Code:** TOE pm **Time Slot/Poster Number:** 03:30

H/D Exchange Levels of Gas Phase Cytochrome c Ions excited in a Linear Quadrupole Ion Trap

JOHN WRIGHT; D.J. Douglas

University of British Columbia, Vancouver, CANADA

Session: Ion Mobility **Code:** TPC **Time Slot/Poster Number:** 041

Ion Mobility - Mass Spectrometry as a Tool for Structural Investigation of High m/z Species

Iain Campuzano¹; Kevin Giles¹; James Langridge¹; Albert Heck²; Cees Versluis²

¹Waters Corporation, Manchester, UNITED KINGDOM; ²Utrecht University, Utrecht, Netherlands

Session: IMS Applications **Code:** TPC **Time Slot/Poster Number:** 052

Evaluating Gas Phase Structure: Coupled H/D Exchange-Ion Mobility Mass Spectrometry

Christopher Becker; Lei Tao; Yiqun Huang; David Russell*

Texas A&M University, College Station, TX

Session: Ion Structures Determined by MS **Code:** TPD **Time Slot/Poster Number:** 065

H/D exchange of deprotonated amino acids and peptides

zhixin tian; Steven R. Kass

Department of chemistry, University of Minnesota, Minneapolis, MN

Session: Ion Mobility **Code:** TPV **Time Slot/Poster Number:** 325

Gas-phase structures of large human transthyretin aggregates: evidence from ion mobility mass spectrometry

Suk-Joon Hyung; Brandon T. Ruotolo; Carol V. Robinson

Department of Chemistry, University of Cambridge, Cambridge, UNITED KINGDOM

Session: Protein Conformation **Code:** TPV **Time Slot/Poster Number:** 326

H/D Exchange Mass Spectrometric Studies of p38 MAP Kinase With Inhibitor SB203580

Susan L. Chen¹; Kyle Asmus²; Melissa Brock²; Sheng Li²; Virgil L. Woods, Jr.²; Roland S. Annan¹

¹GlaxoSmithKline, King of Prussia, PA; ²University of California, San Diego, La Jolla, CA

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 327

Conformational changes and chemical reactivity of the ribosome: An application of limited proteolysis and matrix-assisted laser desorption/ionization mass spectrometry

Daisy-Malloy Hamburg¹; MooJin Suh²; Patrick A. Limbach¹

¹University of Cincinnati, Cincinnati, OH; ²Cornell Weil College Medicine, New York, NY

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 328

Cap-free structure of eIF4E suggests a basis for conformational regulation by its ligands

Nadeem Siddiqui¹; Laurent Volpon¹; Michael J Osborne¹; Ivan Topisirovic¹; Katherine LB Borden¹; Bernard F Gibbs²

¹Dept. of Pathology and Cell Biology, Montreal, Canada; ²Sheldon Biotechnology Center, McGill University, Montreal, Canada

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TPV **Time Slot/Poster Number:** 329

Identification of coactivator binding epitopes on nuclear receptor heterodimer complexes with high resolution hydrogen deuterium exchange mass spectrometry

Scott A. Busby; Michael J. Chalmers; Bruce D. Pascal; Mark R. Southern; Patrick R. Griffin

Scripps Florida, Jupiter, FL

Session: Proteins: Membrane **Code:** TPV **Time Slot/Poster Number:** 330

Exploring Protein-Lipid Interaction by Chemical Cross-linking and Mass Spectrometry

Bill Huang; Hee-Yong Kim

NIAAA/NIH, Rockville, MD

Session: Characterizing Biopolymer Structure and Dynamics **Code:** TPV **Time Slot/Poster Number:** 331

Combining HDX-MS with Molecular Simulations for Drug Discovery

David Schriemer¹; Jack Tuszynski²

¹University of Calgary, Calgary, CANADA; ²University of Alberta, Edmonton, Canada

Session: Characterizing Biopolymer Structure and Dynamics **Code:** TPV **Time Slot/Poster Number:** 333

The binding of human telomeric protein TRF2 to DNA as explored by high resolution PLIMSTEX and novel kinetic modeling.

Justin Sperry¹; Don L. Rempel¹; Xiangguo Shi²; Yoshifumi Nishimura³; Satoko Akashi³; Michael L. Gross¹

¹Washington University in St. Louis, Saint Louis, MO; ²Harvard University, Cambridge, MA; ³Yokohama City University, Tsurumi-ku, Yokohama, Japan

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 334

HXMS reveals conformational and dynamic changes associated with activation of lymphocytic cell kinase by the viral Tip protein

David D. Weis¹; Lori A. Emert-Sedlak²; Thomas E. Smithgall²; John R. Engen³

¹University of New Mexico, Albuquerque, NM; ²University of Pittsburgh, Pittsburgh, PA; ³The Barnett Institute, Northeastern University, Boston, MA

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TPV **Time Slot/Poster Number:** 335

ESI MS study of pepsin inactivation: implications of small-scale protein conformational changes for substrate binding and enzymatic activity

Agya K. Frimpong; Igor A. Kaltashov

University of Massachusetts, Amherst, MA

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 336

Analysis of the pH-dependent pore formation of the protective antigen of anthrax by protein oxidative surface mapping

Joshua S. Sharp¹; Jeffrey F. Kuhn²; Kenneth B. Tomer¹

¹National Institute of Environmental Health Science, RTP, NC; ²Varian, Inc. Scientific Instruments, Cary, NC

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TPV **Time Slot/Poster Number:** 337

Insights into how the "DNA Baton" is passed in the BER Pathway, Mapping APE-1 and DNA Polymerase β contacts

Eizadora Yu; Sara Gaucher; Carmen Pancerella; Ken Sale; Malin Young; Masood Hadi

Sandia National Laboratories, Livermore, CA

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 338

Separation of up to 100 Conformers of Large Protein Ions by FAIMS/MS and Approach to their Structural Attribution

Alexandre A. Shvartsburg¹; Sergei Noskov²; Tadeusz Bryskiewicz³; Randall Purves³; Richard D Smith¹

¹USDoE PNNL, Richland, WA; ²University of Calgary, Calgary, Canada; ³Thermo Electron, Ottawa, Canada

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 339

Structural Studies of Human Bile Acid CoA:Amino Acid N-Acyltransferase (hBAT) Using Hydrogen/Deuterium Exchange

Erin M Shonsey; Matthew B Renfrow; Sebyung Kang; Stephen Barnes

University of Alabama at Birmingham, Birmingham, AL

Session: Characterizing Biopolymer Structure and Dynamics **Code:** TPV **Time Slot/Poster Number:** 340

Domain-Specific Thermodynamic Analysis of Large Multi-Domain Proteins Using SUPREX

Liangjie Tang¹; Konstantin Kazarian²; John C. Williams²; Michael C. Fitzgerald¹

¹Duke University, Durham, NC; ²Thomas Jefferson University, Philadelphia, PA

Session: Protein Conformation **Code:** TPV **Time Slot/Poster Number:** 341

Systematic fragmentation analysis of peptide complexes generated by collision-induced dissociative crosslinking reagents: implications for mass spectrometry-based protein structural studies

Erik J. Soderblom; Michael B. Goshe

North Carolina State University, Raleigh, NC

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 342

Deuterium Labeling in Ubiquitin during Hydrogen/Deuterium Exchange (HDX) and ESI-MS/MS: Scrambled or Sunny-side Up?

Peter L Ferguson; Lars Konermann

University of Western Ontario, London, CANADA

Session: Protein Conformation **Code:** TPV **Time Slot/Poster Number:** 343

Controlled Oxidative Chemical Footprinting of Ribonuclease-S-Protein:S-Peptide Complex by Laser Flash Photolysis of Hydrogen Peroxide.

Brian C. Gau; Michael L. Gross

Washington University, St. Louis, MO

Session: Characterizing Biopolymer Structure and Dynamics **Code:** TPV **Time Slot/Poster Number:** 344

Hydrogen-deuterium exchange provides evidence for presence of mobile water molecules at the MHC-Peptide binding interface

Sachin Patil; Lilly M. Saleena; Hermann von Grafenstein

University of Toledo, Toledo, OH

Session: Protein Conformation **Code:** TPV **Time Slot/Poster Number:** 345

Testing the efficiency and specificity of pepsins from the Antarctic fish *Trematomus bernacchii* for HDX-MS experiments

Sebastien Brier¹; Yan Wu²; Robert Taylor²; Vincenzo Carginale³; Antonio Capasso³; Clemente Capasso³; John R Engen¹

¹The Barnett Institute, Boston, MA; ²Department of Chemistry, University of New Mexico, Albuquerque, NM; ³CNR Institute of Protein Biochemistry, Naples, Italy

Session: MS Characterization of 3D Structure **Code:** TPV **Time Slot/Poster Number:** 346

Probing Tertiary Structure of Bacterial Collagen Binding Domain (CBD) and Catalytic Domain in a multi-domain protein by Limited Proteolysis MALDI-TOF-MS

ROHANA LIYANAGE¹; P. S. T. Leena¹; C. R. Sides¹; Nagarjuna Devarapalli¹; Jennifer Gidden¹; Philominathan O. Matsushita²; J. J. Sakon¹; Jackson O. Lay, Jr¹

¹University of Arkansas, Fayetteville, AR; ²Kagawa Medical University, Miki-cho, Kagawa 761-0793, Japan

Session: MS of Oxidized Proteins **Code:** TPV **Time Slot/Poster Number:** 347

Visualizing actin in the rigor state of the acto-myosin motor by using structural mass spectrometry

J.K. Amisha Kamal¹; Sabrina Benchaar²; Emil Reisler²; Mark chance¹

¹Case Western Reserve University School of Medicine, Cleveland, OH; ²University of California Los Angeles, Los Angeles, CA

Session: What Does MS Tell us about Protein-Protein Interac **Code:** TPV **Time Slot/Poster Number:** 348

MS characterization of serpin and its complex structures

Xiaoqing Zheng; Yuko Tsutsui; Patrick L. Winthrode; Mark R. Chance

case western reserve university, cleveland, OH

Session: Characterizing Biopolymer Structure and Dynamics **Code:** TPV **Time Slot/Poster Number:** 349

DIFFERENTIATION OF BIOLOGICAL ION SHAPES EMPLOYING NANO-ELECTROSPRAY AND ION MOBILITY MASS SPECTROMETRY

Mark Allen¹; John Shockcor²; Rob Plumb²; Alan Miller²; Chris Hughes²; Mark Baumert¹; Jack Henion¹

¹Advion BioSciences, Ithaca, NY; ²Waters, Milford, MA

Session: Characterizing Cross-Linked Proteins with MS **Code:** TPW **Time Slot/Poster Number:** 353

An aptly positioned azido group in a protein cross-linker for facile mapping of amino acids in close proximity

Piotr Kasper; Jaap Willem Back; Maxime Vitale; Alloysius F. Hartog; Winfried Roseboom; Leo J. de Koning; Jan H. van Maarseveen; Anton O. Muijsers; Luitzen de Jong; Chris G. de Koster

University of Amsterdam, Amsterdam, NETHERLANDS

Session: Characterizing Cross-Linked Proteins with MS **Code:** TPW **Time Slot/Poster Number:** 354

Therapeutic protein aggregates: Direct analysis by chemical cross-linking and high-mass MALDI mass spectrometry

Alexis Nazabal; Ryan Wenzel

CovalX AG, ZÄrich, SWITZERLAND

Session: Proteins: General **Code:** TPW **Time Slot/Poster Number:** 355

Cross-Linking and UPLC/MS/MS analysis of the Tif34/Tif35 Protein Complex

Amadeu H Iglesias; Fabio C Gozzo

Brazilian Synchrotron Light Source, Campinas, Brazil

Session: Metal Ions in Biology **Code:** TPW **Time Slot/Poster Number:** 356

Copper Binding of the β -2-Microglobulin Oligomers Studied by Metal-Catalyzed Oxidation Reactions and Mass Spectrometry

Srikanth Rapole; Richard W. Vachet

University of Massachusetts, Amherst, MA

Session: Proteins: General **Code:** TPW **Time Slot/Poster Number:** 357

Investigating Domain Swapping in the C-terminal Domain of the HIV-1 Capsid Protein using Chemical Cross-linking and Mass Spectrometry

Lisa M. Jones; Sebyung Kang; Matthew B. Renfrow; Peter E. Prevelige, Jr.

University of Alabama at Birmingham, Birmingham, AL

Session: Proteins: General **Code:** TPW **Time Slot/Poster Number:** 364

Deuterium exchange mass spectrometry studies of GroupIA PLA2 utilizing novel methods for lipid protein interactions and highly disulfide bound proteins

John Burke¹

¹UCSD, La Jolla, CA; ²University of California San Diego, La Jolla, CA

Session: Proteins: General **Code:** TPW **Time Slot/Poster Number:** 371
A Novel Mass Defect Labeled Mass-Spectrometry Identifiable Cross-linker
Lisabeth L. Hoffman; Ryan M. Phillips; George F. Majetich; I. Jonathan Amster
University of Georgia, Athens, GA

Session: MS of Oxidized Proteins **Code:** TPY **Time Slot/Poster Number:** 400
Oxidation of DNA-binding proteins: from damage to loss of function.
Corinne BurÅ©¹; Nathalie Gillard¹; Stephane Goffinont¹; Marie Davidkova²; FranÅ§oise Culard¹; Melanie Spothem-Maurizot¹; Martine Cadene¹
¹*Centre de Biophysique Moleculaire CNRS UPR4301, ORLEANS, FRANCE*; ²*Nuclear Physics Institute, Prague, Czech Republic*

Session: Proteins: Modified **Code:** TPY **Time Slot/Poster Number:** 411
Characterizing the α,β -Unsaturated Aldehyde Acrolein's Role in the Covalent Cross-Linking of Proteins and Peptides Using Proteomics
Lewis C Jackson; Bert C Lynn
University of Kentucky, Lexington, KY

Session: Proteins: Modified **Code:** TPY **Time Slot/Poster Number:** 415
Probing the conformation and activity of trypsin by amidation labeling
Xiaohui Liu; William C. Broshears; James P. Reilly
Indiana University, Bloomington, IN

Session: Proteomics: Biomarkers **Code:** TPZ1 **Time Slot/Poster Number:** 463
In vivo quantitative interactome analysis of the amyloid precursor protein by time-controlled transcadiac perfusion crosslinking
Yu Bai; Kelly Markham; Fusheng Chen; Rasanjala Weerasekera; Joel Watts; Patrick Horne; Yosuke Wakutani; Gerold Schmitt-Ulms
CRND, University of Toronto, Toronto, CANADA

WEDNESDAY

Session: MS Characterization of 3D Structure **Code:** WOC am **Time Slot/Poster Number:** 08:15

SNAPPshots of Protein Folding: Monitoring Ligand-Induced Folding by Selective Noncovalent Adduct Protein Probing Mass Spectrometry

Ryan R. Julian; Tony Ly

University of California, Riverside, Riverside, CA

Session: MS Characterization of 3D Structure **Code:** WOC am **Time Slot/Poster Number:** 08:35

Ion Mobility Mass Spectrometry and MS/MS of non-covalent protein:carbohydrate complexes indicate conformational differences.

Julie A. Leary¹; Matthew Schenauer¹; Iain Campuzano²; James Langridge²

¹UC Davis, Davis, CA; ²Waters, Inc., Altrincham, United Kingdom

Session: MS Characterization of 3D Structure **Code:** WOC am **Time Slot/Poster Number:** 08:55

DXMS combined with de novo protein structure prediction facilitates model selection

Lars Malmstroem; Liming Hou; William Atkins; David R. Goodlett

University of Washington, Seattle, WA

Session: Proteins: General **Code:** WOC am **Time Slot/Poster Number:** 09:15

Footprinting coupled to UPLC/MS/MS to map the interaction surface between Tif34 and HisTif35 proteins

Fabio C Gozzo; Amadeu H Iglesias

Brazilian Synchrotron Light Source, Campinas, BRAZIL

Session: MS Characterization of 3D Structure **Code:** WOC am **Time Slot/Poster Number:** 09:35

Structure and dynamics of regulatory domains present in retroviral RNA

ARIE HAWKINS¹; Eizadora T. Yu²; Daniele Fabris¹

¹University of Maryland, Baltimore County, Baltimore, MD; ²Sandia National Laboratories, Livermore, CA

Session: Characterizing Cross-Linked Proteins with MS **Code:** WOC am **Time Slot/Poster Number:** 09:55

Protein Structure and Conformation Revealed Using Sequential Cross-linker Rate Measurements (SCRaM): Direct Measurement of Inter-Residue Distances and Secondary Structure

Joseph Schoeniger; Richard Jacobsen; Kenneth Sale

Sandia National Labs, Livermore, CA

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 02:30

Hydrogen / Deuterium Exchange and Crystallography Reveal that Protein Dynamics and Structure Control PPAR gamma Mediated Transcriptional Activity

Michael J. Chalmers; John B. Bruning; Scott A. Busby; Swati Prasad; Bruce D. Pascal; Mark R. Southern; Kendal W. Nettles; Patrick R. Griffin

Scripps Florida, Jupiter, FL

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 02:50

Analysis of Structure in Refolding Intermediates of Indole-3-Glycerol Phosphate Synthase (sIGPS), a TIM barrel protein, by Hydrogen Exchange Mass Spectrometry

Zhenyu Gu; Jill A. Zitzewitz; C. Robert Matthews

University of Massachusetts, Medical School., worcester, MA

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 03:10

Conformation-specific characterization of protein higher order structure using hydrogen exchange and tandem mass spectrometry

Rinat R. Abzalimov; Igor A. Kaltashov

University of Massachusetts, Amherst, MA

Session: Peptide Ion Fragmentation Mechanisms â€” CID and ECD **Code:** WOE pm **Time Slot/Poster Number:** 03:10

Combination of CID and SID with H/D Exchange to Probe the Gas-Phase Intramolecular Rearrangement Process of Protonated Peptides.

Asiri Galhena; Arpad Somogyi; Brittany Perkins; Vicki. H. Wysocki*

University of Arizona, Tucson, AZ

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 03:30
Combining H/D exchange and native electrospray mass spectrometry for unraveling the unfolding mechanism of B.subtilis NAD synthase
Anton Poliakov; Irina Protasevich; Peter E Prevelige; Christie Brouillette
University of Alabama at Birmingham, Birmingham, AL

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 03:50
Oxidative Surface Mapping Generates Biophysical Constraints for Molecular Dynamics Simulations: An Integrated Strategy for Studying the Tanford Transition in Beta-Lactoglobulin
Carlee McClintock¹; Kanan Vyas²; Christine Shook²; Robert L. Hettich¹
¹*Oak Ridge National Lab, Oak Ridge, TN*; ²*University of Tennessee, Knoxville, TN*

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WOC pm **Time Slot/Poster Number:** 04:10
Mapping the structure and dynamics of dark- and light-state bovine rhodopsin by synchrotron radiolysis and high resolution mass spectrometry
Sayan Gupta; Beata Jastrzebska; Rhijuta Dâ€™Mello; Krzysztof Palczewski; Mark Chance
CWRU, Cleveland, OH

Session: MALDI Sample Preparation **Code:** WPC **Time Slot/Poster Number:** 048
Ca²⁺-dependent deuterium exchange properties of EF-hand calcium-binding proteins calmodulin and S100 are useful to monitor MALDI HDX efficiency
Peter L. Pingerelli; Victor V. Ozols; Carly R. Anderson; Richard S. Burns
Barrow Neurological Institute, Phoenix, AZ

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 142
Viral molecular motors visualized by macromolecular mass spectrometry
Kristina Lorenzen¹; Charlotte Uetrecht¹; Adam Oliâ€™a²; Gino Cingolani²; Albert Heck¹
¹*University Utrecht, Biomolecular MS, Utrecht, Netherlands*; ²*SUNY Upstate Medical University, Syracuse, New York*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 143
On the composition of gas-phase ions from protein complexes: contributions to their overall mass
Joanna Freeke; Brandon T. Ruotolo; Adam R. McKay; Carol V. Robinson
University of Cambridge, Cambridge, UK

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 144
ESI-FTMS investigation of the non-covalent interactions between the HIV-1 nucleocapsid protein p7 (NC) and the U5:Aug duplex
Sonnet Davis; Daniele Fabris
University of Maryland Baltimore County, Baltimore, MD

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 145
A Fluorescence Probe of Conformational Dynamics of Non-covalent Complexes in Gas Phase
Xiangguo Shi; Denis Duft; Joel H. Parks
Rowland Institute at Harvard, Cambridge, MA

Session: Ion Trap Applications **Code:** WPJ **Time Slot/Poster Number:** 146
Investigating the stability of various non-covalent macrocycle complexes by energy-variable collision-induced dissociation in a linear ion trap mass spectrometer
Emily Jellen¹; D. Michelle Benoist¹; Benjamin Sims¹; Victor Ryzhov²
¹*Western Carolina University, Cullowhee, NC*; ²*Northern Illinois University, DeKalb, IL*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 147
Influence of Zwitterions on Salt Bridge Stabilization of Single Stranded DNA/Peptide Noncovalent Complexes
Sandra Alves¹; Karine Pionnier¹; Anna Warnet¹; Amina Woods²; Jean-claude Tabet¹
¹*University P. and M. Curie, Paris Cedex 05, FRANCE*; ²*NIDA IRP, NIH, Baltimore, USA*

Session: Non-covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 148

Influence of Surface Composition on the Dissociation of Non-Covalent Protein Complexes by SID

Christopher M. Jones; Richard L. Beardsley; Asiri S. Galhena; Eman M. Basha; Elizabeth Vierling; Vicki H. Wysocki
University of Arizona, Tucson, AZ

Session: Metal Ions in Biology **Code:** WPJ **Time Slot/Poster Number:** 149

ESI-induced Shifts in Metal-Peptide Solution Equilibria

Haritha Mattapalli; Christopher J. Veale; Colin S. Burns; Allison S. Danell
East Carolina University, Greenville, NC

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 150

Phase-Sensitive Detection of Non-Covalent Complexes Using Time Modulated Ligand Delivery

Marites J. Ayson; James S. Brennan; Joseph S. Schoeniger
Sandia National Laboratories, Livermore, CA

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 151

The Specificity of Bacterial Pilus Assembly: Monitoring Subunit-Subunit Interactions using Non-covalent Electrospray Ionisation Mass Spectrometry

Rebecca J Rose¹; Han Remaut²; Denis Verger²; Tina Daviter²; Gabriel Waksman²; Sheena E Radford¹; Alison E Ashcroft¹
¹*University of Leeds, Leeds, UNITED KINGDOM*; ²*Birkbeck College, London, UNITED KINGDOM*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 152

Study of non-covalent complexes between human kinases and clinical inhibitors by nanoESI-MS

MATTHIAS C. JECKLIN¹; David Touboul¹; Paul Ramage²; Rishi Jain³; John Tallarico³; Renato Zenobi¹
¹*ETH Zurich, Zurich, SWITZERLAND*; ²*Novartis Institutes for Biomedical Research, PSU, Basel, Switzerland*; ³*Novartis Institutes for Biomedical Research, GDC, Cambridge, MA, USA*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 153

Screening a Small Dynamic Combinatorial Library for Novel Ribonuclease A Ligands using ESI-FTICR-MS

Michelle M. Sweeney¹; Steven A. Benner²; John R. Eyster¹
¹*University of Florida, Gainesville, FL*; ²*Foundation for Applied Molecular Evolution, Gainesville, FL*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 154

A study of the assembly and disassembly pathways of non-covalent homo-oligomer complexes using nano-ESI-mass spectrometry

ELISABETTA BOERI ERBA¹; Emmanuel Levy²; Helena Hernandez¹; Laura Lane¹; Carol V Robinson¹
¹*University of Cambridge, Department of Chemistry, Cambridge, UNITED KINGDOM*; ²*MRC Laboratory of Molecular Biology, Cambridge, UNITED KINGDOM*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 155

Optimization of In-Line Gel Filtration Conditions for Non-Denaturing Mass Spectrometry

Greg M. Waitt; Jon D. Williams
GlaxoSmithKline, RTP, NC

Session: Using MS to Study the Role of Metal Ions in Biolog **Code:** WPJ **Time Slot/Poster Number:** 156

Platination of superoxide dismutase with cisplatin: Identifying protein platination sites using Fourier transform ion cyclotron resonance mass spectrometry

Stefan K Weidt; C Logan Mackay; Pat R R Langridge-Smith; Peter J Sadler
University of Edinburgh, Edinburgh, UNITED KINGDOM

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 157

Towards Understanding the Effects of Chaotropic Agents on Homo-oligomeric Protein Complexes.

Laura A Lane; Elisabetta Boeri Erba; Helena Hernandez; Carol V Robinson
University of Cambridge, Cambridge, UNITED KINGDOM

Session: Non-covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 158

Automated Online Real-time Nano-MS Reaction Monitoring and its Application to Non-covalent Protein Complex Dynamics and Kinetics

Alexander James Painter; Justin LP Benesch; Carol V Robinson
Cambridge University, Cambridge, United Kingdom

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 159

Online Mass Spectrometric Investigation of Chiral Amplification of Amino Acid Sublimates

Marcela Nefliu¹; Richard H. Perry¹; Chunping Wu¹; Sean Bird²; David E. Clemmer²; R. Graham Cooks¹
¹*Purdue Univ., West Lafayette, IN*; ²*Indiana Univ., Bloomington, IN*

Session: What Does MS Tell us about Protein-Protein Interac **Code:** WPJ **Time Slot/Poster Number:** 160

Sulfation, its role and mechanism in protein-protein interaction

Amina S. Woods; Shelley N. Jackson
NIDA IRP, NIH, Baltimore, MD

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 161

Techniques for improved analysis of noncovalent protein complexes on the QSTAR® Elite quadrupole time-of-flight system

Douglas A. Simmons
MDS Sciex, Concord, CANADA

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 162

[Determination of non-covalent interactions between antisense oligonucleotides and Î²âˆ²-cyclodextrin using electrospray ionization mass spectrometry

James A McKee; Catherine Bentzley
University of the Sciences in Philadelphia, Philadelphia, PA

Session: Non-covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 163

Mapping binding sites of nucleic acid ligands targeting unique structural features of the HIV-1 polypurine tract by tandem mass spectrometry

Kevin B. Turner¹; Robert Brinson²; Hye Young Yi-Brunozzi³; Jason W. Rausch³; John P. Marino²; Stuart F. J. Le Grice³; Daniele Fabris¹
¹*University of Maryland Baltimore County, Baltimore, MD*; ²*University of Maryland Biotechnology Institute, Rockville, MD*; ³*NCI, National Institutes of Health, Frederick, MD*

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 164

Investigation of non-covalent DNA/drug complex by FT/ICR

Ying Xu¹; Afonso Carlos¹; FranÃ§oise Fournier¹; Ren Wen²; Jean-claude Tabet¹
¹*University P. and M. Curie, Paris Cedex 05, FRANCE*; ²*Fudan University, Shanghai, China*

Session: What Does MS Tell us about Protein-Protein Interac **Code:** WPJ **Time Slot/Poster Number:** 165

Quaternary structure of multiprotein complexes defined by ES-MS. Not all complexes are created equal

Jiangxiao Sun; Nian Sun; Elena Kitova; John Klassen
University of Alberta, Edmonton, CANADA

Session: Non-Covalent Interactions **Code:** WPJ **Time Slot/Poster Number:** 166

DNA stabilization by noncovalent polynuclear platinum phosphate clamps

John B. Mangrum; Nicholas P. Farrell
Virginia Commonwealth University, Richmond, VA

Session: Bioinformatics **Code:** WPQ **Time Slot/Poster Number:** 262 **Software for the determination of backbone amide deuterium levels from H/D exchange MS data**

Bruce D. Pascal; Michael J. Chalmers; Scott A. Busby; Christopher C. Mader; Mark R. Southern; Nicholas F. Tsinoremas; Patrick R. Griffin
The Scripps Research Institute, Jupiter, FL

Session: IMS Instrumentation **Code:** WPZ1 **Time Slot/Poster Number:** 432

Probing the structures of defensin antimicrobial peptides by Ion Mobility and Gas Phase Hydrogen/Deuterium Exchange Mass Spectrometry

Wutharath Chin
University of Edinburgh, Edinburgh, UNITED KINGDOM

Session: Nucleic Acids **Code:** WPZ2 **Time Slot/Poster Number:** 439

Characterization of Nucleic Acid Secondary Structure by Gas-phase H/D Exchange in a Q-FT-ICR Mass Spectrometer

Jingjie Mo; Kristina Håkansson

University of Michigan, Ann Arbor, MI

Session: Nucleic Acids **Code:** WPZ2 **Time Slot/Poster Number:** 442

Identification of Oligonucleotide-Peptide Cross-links using Mass Defect Scans

Soheil Pourshahian; Patrick A Limbach

University of Cincinnati, Cincinnati, OH

Session: Nucleic Acids **Code:** WPZ2 **Time Slot/Poster Number:** 453

Title: Probing the conformations of the 5'UTR riboswitch of HIV-1 using crosslinking reagents and ESI-FTICR mass spectrometry

Dong Yang; Daniele Fabris

University of Maryland, Baltimore County, Baltimore, MD

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WPZ3 **Time Slot/Poster Number:** 455

Exploring Trp-Cage Configurations both in the Dry and when Wet

Perdita Barran; Jason Kalapothakis ; Claire MacMillan; Bryan McCullough

The University of Edinburgh, Edinburgh,

Session: Proteins: Folding **Code:** WPZ3 **Time Slot/Poster Number:** 456

Using Mass Spectrometry-based Hydrogen/Deuterium Exchange for the Optimization of Protein Constructs in NMR Structure Determination

Seema Sharma; Haiyan Zheng; Li-chung Ma; Janet Huang; Peter Lobel; Gaetano T. Montelione

CABM, Rutgers University, Piscataway, NJ

Session: ESI in the year of John Fenn's 90th Birthday **Code:** WPZ3 **Time Slot/Poster Number:** 457

Signal Response of Co-Existing Protein Conformers in Electrospray Ionization Mass Spectrometry

Mark C. Kuprowski; Lars Konermann

University of Western Ontario, London, CANADA

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WPZ3 **Time Slot/Poster Number:** 458

The first step of hen egg white lysozyme fibrillation, irreversible partial unfolding, studied by ESI MS.

Ming Xu²; Viktor A. Shashilov²; Vladimir V. Ermolenkov²; Laura Fredriksen²; Igor K. Lednev²; DMITRI ZAGOREVSKI¹

¹Rensselaer Polytechnic Institute, Troy, NY; ²University at Albany, SUNY, Albany, NY

Session: LC/MS **Code:** WPZ3 **Time Slot/Poster Number:** 459

The structure of human prion protein amyloid fibrils determined by hydrogen exchange-mass spectrometry

Xiaojun Lu; Patrick L. Wintrode; Witold K. Surewicz

Case Western Reserve University, Cleveland, OH

Session: ESI in the year of John Fenn's 90th Birthday **Code:** WPZ3 **Time Slot/Poster Number:** 460

Protein Folding Studied by ESI-MS: Insights into the Relationship between Protein Conformation and Charge State Distribution from Molecular Dynamics Simulations

LARS KONERMANN

University of Western Ontario, London, CANADA

Session: Proteins: Membrane **Code:** WPZ3 **Time Slot/Poster Number:** 461

Mechanism of the insertion of bilayer membrane by melittin

Kazumi Saikusa

Graduate school of science, Hiroshima University, Higashihiroshima, JAPAN

Session: Peptide Ion Fragmentation Mechanisms " CID and ECD **Code:** WPZ3 **Time Slot/Poster Number:** 462

Probing the Gas Phase Folding Kinetics of Peptide Ions by IR Activated DR-ECD

CHENG LIN; JASON J. COURNOYER; PETER B. O'CONNOR

Boston University, Boston, MA

Session: Characterizing Biopolymer Structure and Dynamics **Code:** WPZ3 **Time Slot/Poster Number:** 463

Temperature-dependent Hydrogen/Deuterium Exchange is an indispensable tool for characterizing ALS mutant SOD1 proteins.

Armando Durazo¹; Bryan F. Shaw²; Kym F. Faul¹; Julian P. Whitelegge¹; Joan S. Valentine¹

¹UCLA, Los Angeles, CA; ²Harvard, Cambridge, MA

Session: MS in the Determination of Cellular Pathways **Code:** WPZ3 **Time Slot/Poster Number:** 464

Ex Vivo Analysis of Protein-Ligand Binding Interactions in Cellular Pathways using SUPREX

Petra L. Roulhac¹; Katherine D. Weaver¹; Timothy A. Mietzner²; Cynthia N. Cornelissen³; Alvin L. Crumbliss¹; Michael C. Fitzgerald¹

¹Duke University, Durham, NC; ²University of Pittsburgh, Pittsburgh, PA; ³Virginia Commonwealth University, Richmond, VA

THURSDAY

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 08:15

Noncovalent interactions between alkali cations and amino acids: Effects of the side chain

Peter B. Armentrout; Amy Heaton; Sha Ye; Robert M. Moision; Amy Clark

University of Utah, Salt Lake City, UT

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 08:35

Experimental and Theoretical Studies of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues Peptides

Zhibo Yang; Julia Laskin

Pacific Northwest National Laboratory, Richland, WA

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 08:55

Mass Spectrometry, Electron Affinities and non-covalent interactions of DNA bases and base pairs.

EDWARD C CHEN; Edward S. Chen

University of Houston, Houston, TX

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 09:15

Noncovalent Binding Constants Determined by Mass Spectrometric Methods: Current Status, Limitations, and Future Prospects

Renato Zenobi; CÄ©dric Bovet; Matthias Jecklin; Sonal Mathur; David Touboul; Arno Wortmann

ETH Zurich, Zurich, SWITZERLAND

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 09:35

Detection and Quantification of siRNA double strands by MALDI-MS

Michael Karas¹; Ute Bahr¹; HÄ¼seyin AygÄ¼n²

¹*JW Goethe Univ. of Frankfurt, Frankfurt am Main, GERMANY;* ²*BioSpring, Frankfurt, Germany*

Session: Non-covalent Interactions **Code:** ThOC am **Time Slot/Poster Number:** 09:55

Equivalency of binding sites in protein-ligand complexes revealed by time-resolved tandem mass spectrometry

Glen K. Shoemaker¹; Elena N. Kitova¹; Monica M. Palcic²; John S. Klassen¹

¹*University of Alberta, Edmonton, CANADA;* ²*Carlsberg Laboratory, Copenhagen, Denmark*

Session: MS in the Determination of Cellular Pathways **Code:** ThOA pm **Time Slot/Poster Number:** 03:30

Proteomic and Genomic Analysis of Nuclear Receptor Signaling Pathways

Patrick R Griffin; Jennifer Caldwell Busby; Scott A Busby; Valerie Cavett; Michael J Chalmers; Bruce D Pascal; Swati Prasad; Layton H Smith; Mark R Southern

The Scripps Research Institute, Jupiter, FL

Session: MS of Oxidized Proteins **Code:** ThOE pm **Time Slot/Poster Number:** 02:30

Three-dimensional structure of cofilin bound to monomeric actin derived by structural mass spectrometry data

J.K. Amisha Kamal¹; Sabrina Benchaar²; Keiji Takamoto¹; Emil Reisler²; Mark Chance¹

¹*Case Western Reserve University, Cleveland, OH;* ²*University of California Los Angeles, Los Angeles, CA*

Session: Invited Presentation **Code:** ThOE pm **Time Slot/Poster Number:** 03:10

Characterization of Electrochemical-Induced Protein Oxidation as a Probe for Higher Order Protein Structural Interrogation

Robert Hettich; Carlee McClintock; Vilmos Kertesz

Oak Ridge National Laboratory, Oak Ridge, TN

Session: Ion Structures Determined by MS **Code:** ThOG pm **Time Slot/Poster Number:** 03:10

Hydrogen/Deuterium Exchange of Alanine Oligomeric Peptides: A Case Study of HAAAA

Brittany R. Perkins; Kristin A. Herrmann Favela; Linda Breci; Vicki Wysocki

Chemistry Department, University of Arizona, Tucson, AZ

Session: MS of Oxidized Proteins **Code:** ThOE pm **Time Slot/Poster Number:** 03:30

Probing oxidative stress using intact protein LC-MS

Ljiljana Pasa-Tolic; Natacha M. Lourette; Heather S. Smallwood; Si Wu; Curt B. Boschek; Thomas C. Squier; Richard D. Smith
Pacific NW Nat'l Lab, Richland, WA

Session: Ion Structures Determined by MS **Code:** ThOG pm **Time Slot/Poster Number:** 03:30

Shedding light on the structures of CID and HDX product ions

Nick C Polfer¹; Bela Paizs²; John R Eyler³; Rob C Dunbar⁴; Jos Oomens⁵

¹Fritz-Haber-Institut, Berlin, Germany; ²German Cancer Research Center, Heidelberg, Germany; ³University of Florida, Gainesville, FL; ⁴Case Western University, Cleveland, OH; ⁵FOM Institute 'Rijnhuizen', Nieuwegein, NETHERLANDS

Session: MS of Oxidized Proteins **Code:** ThOE pm **Time Slot/Poster Number:** 03:50

In Vivo Protein Targets Of Reactive Lipid Peroxidation Products

Juan Chavez; Bingnan Han; Jan F. Stevens; CLAUDIA S. MAIER
Oregon State University, Corvallis, OR

Session: MS of Oxidized Proteins **Code:** ThOE pm **Time Slot/Poster Number:** 04:10

Towards the proteomic mapping of endogenous sites of HNE modification: A two-step solid-phase enrichment strategy for HNE-modified peptides

Mikel R Roe; Hongwei Xie; Juan Feng; Danni L Meany; LaDora V Thompson; Edgar A Arriaga; Timothy J Griffin
University of Minnesota, Minneapolis, MN

Session: What Does MS Tell us about Protein-Protein Interac **Code:** ThPE **Time Slot/Poster Number:** 068

Investigating the effects of the HIV-1 nucleocapsid protein on RNA isomerization by tandem mass spectrometry

KEVIN B. TURNER¹; Nathan A. Hagan²; Daniele Fabris¹

¹University of Maryland Baltimore County, Baltimore, MD; ²Johns Hopkins University, APL, Laurel, MD

Session: Reaction Intermediates **Code:** ThPE **Time Slot/Poster Number:** 072

Mechanisms of Cross-linking Reactions of Genipin with β -Lactoglobulin and Related Peptides by MALDI-TOF/TOF Mass spectrometry

ALBERTO NUNEZ; Phoebe Qi
USDA-ARS-ERRC, Wyndmoor, PA

Session: Carbohydrats/Oligosaccharides **Code:** ThPT **Time Slot/Poster Number:** 326

Structural Characterization of a Short Interfering RNA Duplex by Non-Denaturing Ion-Pair Reversed-Phase HPLC Electrospray Ionization Mass Spectrometry

Scott A. Young; Marsha Langhorst; Mike Fazio; Krishna Kuppannan
The Dow Chemical Company, Midland, MI

Session: Proteomics: Phosphorylation **Code:** ThPY **Time Slot/Poster Number:** 407

2D-nanoLC approach using TiO2 columns for the enrichment of protein-RNA cross-links and phosphopeptides derived from ribonucleoprotein particles for MS-based identification

Florian Richter; Eva KÄ¼hn-HÄ¼lsken; Mads Gronborg; Monika Raabe; Uwe Plessmann; Henning Urlaub
Max Planck Institute for Biophysical Chemistry, Goettingen, GERMANY

Session: Proteomics: Labeling and Affinity **Code:** ThPZ3 **Time Slot/Poster Number:** 484

Application of the Cross-Linker Based Protein Interaction Reporter Technology to *Saccharomyces cerevisiae*

Natalia L. Zakharova¹; Gerhard R. Munske¹; Gordon A. Anderson²; Nikola Tolic²; Xiaoting Tang¹; James E. Bruce¹

¹Washington State University, Pullman, WA; ²Pacific Northwest National Laboratory, Richland, WA

Session: Proteomics: Labeling and Affinity **Code:** ThPZ3 **Time Slot/Poster Number:** 485

Biotinylation and MS Analysis: A Combined Approach for the Identification of the Surface Exposed Residues of Hsp90

Wendell P. Griffith¹; Xueguang Lui²; Dwella M. Nelson¹; Jennifer S. Isaacs²; Robert J. Cotter¹

¹Johns Hopkins School of Medicine, Baltimore, MD; ²Medical University of South Carolina, Charleston, SC

NOTES: