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

FRIDAY, JANUARY 21

6:00 – 7:00 pm **Registration**, *Outside of the Long/Bird/Indian Ballroom*

7:00 – 8:00 pm
Opening Session
Session Chair, Béla Paizs, *DKFZ, Heidelberg*
Long/Bird/Indian Ballroom

7:10 – 8:00 pm **Opening Lecture: Matthias Mann**, *Max-Planck Institute for Biochemistry* "Historical development and current status of peptide identification in proteomics research"

8:00 - 10:00 pm
Reception
setup all posters
Citrus/Glades/Jasmine/Palm rooms

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SATURDAY, JANUARY 22

7:30 – 8:30 am	**Continental Breakfast**, *Citrus/Glades/Jasmine/Palm*

8:30 – 12:00 am
Overview Lecture & Chemistry of CID
Session Chair: Vicki H. Wysocki, *University of Arizona*
Long/Bird/Indian Ballroom

8:30 – 9:00 am	**Béla Paizs**, *DKFZ, Heidelberg* “Peptide Fragmentation Models and Sequencing Strategies”
9:00 – 9:30 am	**Simon Gaskell**, *Queen Mary University of London* “Studies of Peptide CID Using Isotope Labeling and Combined Ion Mobility/MS“
9:30 – 10:00 am	**Gary L. Glish**, *University of North Carolina, Chapel Hill* “Probing Peptide Structure with "Slow Heating" Methods: When CID and IRMPD Give Different Results”
10:00 – 10:30 am	**Coffee Break,** *Citrus/Glades/Jasmine/Palm*
10:30 – 11:00 am	**Gavin Reid**, *Michigan State University, East Lansing* “The Effect of Post-translational and Process-induced Modifications on the Gas-Phase Fragmentation Reactions of Protonated Peptides”
11:00 – 11:30 am	**Stephen E. Stein**, *NIST, Gaithersburg* “Exploring Peptide Fragmentation Using Spectral Libraries”
11:30 – 12:00 am	**Roman Zubarev**, *Karolinska Institutet, Stockholm* “Fragmentomics: Probing Fragmentation Mechanisms by Statistical Analysis of Proteomics Data”
12:00 – 1:30 pm	**Group Lunch,** *Garden Courtyard*

1:30 pm – 4:10 pm
Chemistry of ECD/ETD
Session Chair: Scott McLuckey, *Purdue University*
Long/Bird/Indian Ballroom

1:30 – 2:00 pm	**Frank Tureček**, *University of Washington, Seattle* “Charge Tags, Electron Predators, and Other Toys to Play the Electron Game”
2:00 – 2:30 pm	**Helen Cooper**, *University of Birmingham* “The effect of post-translational modifications on the electron capture/transfer dissociation of peptide ions”
2:30 – 3:00 pm	**Kristina Håkansson**, *University of Michigan* “Negative Ion Electron Capture Dissociation (niECD): Where does the Electron Go?”
3:00 – 3:10 pm	**Short Coffee Break,** *in back of Long/Bird/Indian*
3:10 – 3:40 pm	**Vicki Wysocki**, *University of Arizona* “Characterization of Peptides and Proteins with a Modified Synapt G2”
3:40 – 4:10 pm	**Joshua J. Coon**, *University of Wisconsin, Madison* “How to combine electrons, photons, and collisions for large-scale protein sequencing and quantification”

SATURDAY, JANUARY 22

6:00 – 8:00 pm
Hot Topics I
Session Chair: Gary L. Glish, *University of North Carolina, Chapel Hill*
Long/Bird/Indian Ballroom

6:00 – 6:15 pm	**Peter B. Armentrout,** *University of Utah* “Energetics of the Decomposition of Protonated Glycine, Diglycine, and the Simplest b_2 Ion”
6:15 – 6:30 pm	**Benjamin J. Bythell**, *National High Magnetic Field Laboratory* “Stability of Sequence Ions Generated in Tandem Mass Spectrometry Experiments”
6:30 – 6:45 pm	**Michael van Stipdonk**, *Wichita State University* “Energetics of Protonated Peptide Fragmentation Measured by Threshold Collision-Induced Dissociation”
6:45 – 7:00 pm	**Shabaz Mohammed**, *Utrecht University* “Characterising the Behaviour of Lys-N peptides in Tandem Mass Spectrometry”
7:00 – 7:15 pm	**Ann Westman-Brinkmalm**, *Sahlgrenska University Hospital* "Investigation of database search tools and parameters for identification of endogenous CNS peptides/proteins analyzed by an online top-down MS approach"
7:15 – 7:30 pm	**Hongqian Yang**, *Karolinska Institutet* “Proteome-wide detection and quantification of isoaspartyl residues by ETD FTMS”
7:30 – 7:45 pm	**Meng-Qiu Dong**, *National Institute of Biological Sciences, Beijing* “Improved Peptide Identification for Proteomic Analysis Based on Comprehensive Characterization of Electron Transfer Dissociation Spectra”
7:45 – 8:00 pm	**Weidong Cui,** *Washington University, St. Louis* “Characterization of Intact Protein Complexes by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry”

8:00 - 10:00 pm
Poster Session & Reception
even-number posters will be presented
Citrus/Glades/Jasmine/Palm rooms

SUNDAY, JANUARY 23

7:30 – 8:30 am	**Continental Breakfast**, *Citrus/Glades/Jasmine/Palm*

8:30 – 10:30 am
***de novo* Sequencing of Peptides**
Session Chair: Neil Kelleher, *Northwestern University, Evanston, IL*
Long/Bird/Indian Ballroom

8:30 – 9:00 am	**Pavel Pevzner**, *University of California, San Diego* "When will *de novo* Peptide Sequencing Substitute MS/MS Database Search?"
9:00 – 9:30 am	**Bernhard Spengler**, *Justus Liebig University Giessen* "Accurate mass and *de novo* sequencing strategies for peptide identification and characterization"
9:30 – 10:00 am	**Annette Michalski**, *Max-Planck Institute for Biochemistry, Martinsried* "Improving *de novo* sequencing performance with high dynamic range HCD data"
10:00 – 10:30 am	**Bin Ma**, *University of Waterloo, Waterloo* "Post *De Novo* Sequencing Analyses"
10:30 – 11:00 am	**Coffee Break,** *Citrus/Glades/Jasmine/Palm*

11:00 am – 1:00 pm
Peptide Identification via Database Search
Session Chair: Pavel Pevzner, *University of California, San Diego*
Long/Bird/Indian Ballroom

11:00 – 11:30 am	**Marshall Bern**, *Palo Alto Research Center* "Algorithmic ideas for improving database search"
11:30 – 12:00 am	**William Stafford Noble**, *University of Washington, Seattle* "Machine learning methods for analyzing shotgun proteomics data"
12:00 – 12:30 am	**Ronald Beavis**, *The University of British Columbia, Vancouver* "Annotating Spectrum Libraries and Algorithm Validation"
12:30 – 1:00 pm	**Alexey I. Nesvizhskii**, *University of Michigan, Ann Arbor* "Computational analysis of MS/MS database search results"
1:00 - 6:00 pm	**Afternoon Free**

SUNDAY, JANUARY 23

6:00 – 8:00 pm
Vendor Workshop & Hot Topics II
Session Chair: Bernhard Spengler, *Justus Liebig University Giessen*
Long/Bird/Indian Ballroom

6:00 – 6:15 pm	**Shannon Cornett**, *Bruker Daltonics* “MALDI top-down-sequencing strategy for *de novo* sequencing of an intact 13.6 kDa protein”
6:15 – 6:30 pm	**John Cottrell**, *Matrix Science Ltd.* “Hierarchical Clustering of Shotgun Proteomics Data”
6:30 – 6:45 pm	**Martha Stapels**, *Waters Corporation* “An Unbiased Approach to Increasing Proteome Coverage Using Ion Mobility with MS^E”
6:45 – 7:00 pm	**Robert B. Cody**, *JEOL USA, Inc.* “High-Energy CID: A Lost Art Rediscovered?”
7:00 – 7:15 pm	**Peng Zhao**, *University of Georgia* “Combining HCD and ETD to determine sites of O-GlcNAc modification”
7:15 – 7:30 pm	**Helene L Cardasis**, *Merck Research Labs* “Identification and characterization of endogenous peptides in CSF and plasma using high resolution ETD”
7:30 – 7:45 pm	**Katharina Kramer**, *Max Planck Institute for Biophysical Chemistry* “Investigation of protein-RNA cross-linking by mass spectrometry”
7:45 – 8:00 pm	**Bruce Southey**, *University of Illinois at Urbana Champaign* “Factors influencing neuropeptide identification in a database search”

8:00 - 10:00 pm
Poster Session & Reception
odd-number posters will be presented
Citrus/Glades/Jasmine/Palm rooms

MONDAY, JANUARY 24

7:30 – 8:30 am **Continental Breakfast**, *Citrus/Glades/Jasmine/Palm*
Remove all posters by 1:30 pm

8:30 – 10:00 am
Peptides with PTMs
Session Chair: Gavin Reid, *Michigan State University, East Lansing*
Long/Bird/Indian Ballroom

8:30 – 9:00 am **Ole Jensen**, *University of Southern Denmark, Odense*
"Utility of Various MS/MS Technologies for Protein Identification and Assignment of PTMs in Proteins"

9:00 – 9:30 am **Nathalie Ahn**, University of Colorado at *Boulder, Boulder*
"Evaluating Peptide Identifications using Simulated MS/MS"

9:30 – 10:00 am **Kati Medzihradszky**, *University of California San Francisco*
"MS/MS analysis of sulfo- and glycopeptides: a practical view"

10:00 – 10:30 am **Coffee Break,** *Citrus/Glades/Jasmine/Palm*

10:30 am – 12:30 pm
Perspectives and New Directions
Session Chair: Roman Zubarev, *Karolinska Institutet, Stockholm*
Long/Bird/Indian Ballroom

10:30 – 11:00 am **Scott McLuckey**, *Purdue University, West Lafayette*
"The Roles of Ion-Type and Activation Conditions in the Structural Characterization of Peptide and Protein Ions via MS/MS: Challenges and Possibilities"

11:00 – 11:30 am **Neil Kelleher**, *Northwestern University, Evanston, IL*
"Why do peptides/proteins ~8 kDa and bigger retain phosphorylation during threshold MS/MS techniques like CID**?**"

11:30 am – 12:00 pm **Philippe Maitre**, *Université Paris-Sud 11, Paris*
"Structural characterization of peptide fragments via infrared spectroscopy"

12:00 – 12:30 pm **Jürgen Cox**, *Max-Planck Institute for Biochemistry, Martinsried*
"Putting it all together: In depth informatics and bioinformatic proteome characterization from high resolution mass spectrometric data"

12:30 – 1:00 pm **Closing Remarks**
Béla Paizs & Matthias Mann

Poster List

All posters are located in the Citrus/Glades/Jasmine/Palm rooms
even-number posters will be presented on Saturday from 8:00 - 10:00 pm
odd-number posters will be presented on Sunday from 8:00 - 10:00 pm

1 **Comparison of Fragmentation Patterns in ESI-CID-FTICR, ESI-ECD-FTICR, and MALDI-TOFTOF Mass spectrometry Performed on Endogenous Amyloid β Peptides from Cerebrospinal Fluid;** Gunnar Brinkmalm, Erik Portelius, Henrik Zetterberg, Kaj Blennow, and Ann Westman-Brinkmalm; *Institute of Neuroscience and Physiology, The Sahlgrenska Academy at University of Gothenburg, Sahlgrenska University Hospital, Mölndal, Mölndal, Sweden*

2 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Energetics of the Decomposition of Protonated Glycine, Diglycine, and the Simplest b_2 Ion;** Sha J. Ye, Amy Heaton, Amy Clark, and P. B. Armentrout; *Department of Chemistry, University of Utah*

3 **In Search of Microorganism-Typic Peptides : In-Depth Whole Cell Protein/Peptide Profiling; MS-Experiments for the Accurate Identification of Microorganisms Out of a Mixture;** René Brunisholz[1], Britta Stoop[2], Simone Wüthrich[1], Ralph Schlapbach[1], Frank Hesford[2] and David Drissner[2;] [1]*Functional Genomics Center Zurich, University / ETH Zurich, Zurich;* [2]*Agroscope Changins-Wädenswil Research Station ACW, Food Microbiology and Wine Analytics, Schloss, Wädenswil*

4 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Stability of Sequence Ions Generated in Tandem Mass Spectrometry Experiments;** Benjamin J. Bythell[a], Christopher L. Hendrickson[a,b], Alan G. Marshall[a,b]; [a] *Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Florida State University;* [b]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

5 *Promoted poster 15 minute oral presentation during the Sunday Hot Topics II session* - **Identification and Characterization of Endogenous Peptides in CSF and Plasma Using High Resolution ETD;** Helene L Cardasis, James P. Conway, Nathan A. Yates, and Ronald C. Hendrickson; *Proteomics Department, Merck Research Labs, Rahway, NJ*

6 **The Effect of Timescale on b-ion Rearrangement during Collision Induced Dissociation (CID);** Ross Chawner[1], Simon J. Gaskell[2] and Claire E. Eyers[1]; [1]*Michael Barber Centre for Mass Spectrometry, Manchester Interdisciplinary Biocentre, Manchester, UK;* [2]*Queen Mary University of London, London, UK*

7 **Tandem MS Analysis of Selenamide-Derivatized Peptide/Protein Ions;** Yun Zhang[1], Hao Zhang[2], Weidong Cui[2], Michael L. Gross[2] and Hao Chen[1]*; [1]*Center for Intelligent Chemical Instrumentation, Department of Chemistry and Biochemistry, Ohio University, Athens, OH;* [2]*Department of Chemistry, Washington University in St. Louis, St. Louis, MO*

8 **Top-Down Pseudo MS^3 Analysis of a Native Disulfide-Bonded Protein: Fragmentation Characteristics in Absence of Mobile Protons and Application for Protein Identification via Database Search;** Jianzhong Chen,[1,2] Pavel Shiyanov,[1] John J Schlager,[1] and Kari B Green-Church[2;] [1] *Applied Biotechnology Branch, Air Force Research Laboratory, Dayton, OH;* [2] *Mass Spectrometry and Proteomics Facility, The Ohio State University, Columbus, OH*

9 *Promoted poster 15 minute oral presentation during the Sunday Vendor Workshop session* - **High-Energy CID: A Lost Art Rediscovered?** Robert B. Cody and A. John Dane; *JEOL USA, Inc., Peabody, MA*

10 **Comparison of Peptide Fragmentation using ETD and HCD on Lys-C Generated Peptides;** Karl R. Clauser, Namrata D. Udeshi, and Steven A. Carr; *Broad Institute of MIT and Harvard, Cambridge, MA*

11 *Promoted poster 15 minute oral presentation during the Sunday Vendor Workshop session* - **MALDI Top-Down-Sequencing Strategy for *de novo* Sequencing of an Intact 13.6 kDa Protein;** Shannon Cornett, Anja Resemann, Dirk Wunderlich, Jens Fuchser, Detlev Suckau; *Bruker Daltonics, Billerica, MA*

12 **Mapping Proton Distribution using Electron Capture Dissociation;** David M. Crizer, Natalie J. Thompson, Takashi Baba, and Gary L. Glish; *University of North Carolina, Chapel Hill, NC*

13 *Promoted poster 15 minute oral presentation during the Sunday Vendor Workshop session* - **Hierarchical Clustering of Shotgun Proteomics Data;** Ville Koskinen, David Creasy, and John Cottrell; *Matrix Science Ltd., London UK*

14 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Characterization of Intact Protein Complexes by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Weidong Cui, Hao Zhang, Jianzhong Wen, Robert E. Blankenship, and Michael L. Gross; *Washington University, St. Louis, MO*

15 **Isolation and Identification of the Primary Structure of a Mannose-Binding Lectin from the Serum of the American Alligator (*Alligator mississippiensis*);** Lancia Darville[1], Mark Merchant[2] and Kermit Murray[1]; *[1]Louisiana State University, Baton Rouge, LA, [2]McNeese State University, Lake Charles, LA*

16 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Improved Peptide Identification for Proteomic Analysis Based on Comprehensive Characterization of Electron Transfer Dissociation Spectra;** Rui-Xiang Sun[1*], Meng-Qiu Dong[2*], Chun-Qing Song[2], Hao Chi[1], Bing Yang[2], Li-Yun Xiu[1], Li Tao[2], Zhi-Yi Jing[2], Chao Liu[1], Le-Heng Wang[1], Yan Fu[1], and Si-Min He[1]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing China; [2] National Institute of Biological Sciences, Beijing China*

17 **Characterizing Extracellular Protein Post-translational Modifications in Cellulose-Degrading Bacteria by a Combined CAD and ETD Approach;** Andrew B. Dykstra[1,2], Babu Raman[1], Kelsey D. Cook[2], Robert L. Hettich[1]; *[1]Oak Ridge National Lab, Oak Ridge, TN, [2]University of Tennessee, Knoxville, TN*

18 **The Influence of a_n and a_n-17 Ions on Peptide Dissociation Pathways;** Alessandra L. Ferzoco[1], Sandra E. Spencer[1], Meredith L. Arnold[1], Jeffrey Steill[2], Jos Oomens[2], and Gary L.Glish[1]; *[1]University of North Carolina, Chapel Hill, NC; [2]FOM Institute for Plasmaphysics Rijnhuizen, Nieuwegein, Netherlands*

19 **Assessment of Protein Translation in Yeast through Amino Terminal Peptide Identification;** Claire Fournier[1], Justin Cherny[1], Kris Truncali[1,2], Danny Krizanc[2], Michael Weir[1]; *[1]Department of Biology, [2]Department of Mathematics and Computer Science, Wesleyan University*

20 **An Algorithm for Identifying Multiply-Modified Endogenous Proteins using both Full-Scan and High Resolution MS/MS Data;** Ray Fyhr[1] and Matthew T. Mazur[2,]; *[1] Department of Information Technology, [2] Department of Proteomics, Merck Research Laboratories, Rahway, NJ*

21 **Multiple-Stage CID Fragmentation of Cyclic Peptides Containing Arg and Lys Residues;** Fuyu Guan [a], Cornelius E. Uboh [a,b], and Lawrence R. Soma [a]; **[a]** *School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA;* **[b]** *PA Equine Toxicology and Research Center, West Chester University, West Chester, PA*

22 **Structural Studies of Histidine and Proline-containing b_2^+ Peptide Fragment Ions;** Ashley C. Gucinski,[1,2] Arpad Somogyi,[1] Julia Chamot-Rooke,[2] Unige A. Laskay,[1] and Vicki H. Wysocki[1]; *[1]Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ; [2] Laboratoire des Mecanismes Reactionnels, Ecole Polytechnique, Palaiseau, France*

23 **Towards *de novo* Sequencing of Entire Proteins via Iterative Shotgun Protein Sequencing;** Adrian Guthals[1], Karl Clauser[2], Nuno Bandeira[1,3,4]; [1] *Dept. Computer Science and Engineering, UCSD;* [2] *Broad Institute of MIT and Harvard;* [3] *Skaggs School of Pharmacy and Pharmaceutical Sciences, UCSD;* [4] *Center for Computational Mass Spectrometry, UCSD*

24 **N-Protonated Isomers Are the Gateways to Peptide Ion Fragmentation;** Fredrik Haeffner and Karl K. Irikura; *Computational Chemistry Group, Chemical and Biochemical Reference Data Division, Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD*

25 **Fragmentation Properties of Non-Tryptic Native Peptides using CID and ETD;** Sarah R. Hart; *Keele University School of Medicine, Keele, Staffordshire, UK*

26 **Use of AQUA and MALDI-TOF/TOF MS to Quantify a Dioxin-Degrading Enzyme;** Erica M. Hartmann and Rolf U. Halden[1,2]; [1]*The Biodesign Institute at Arizona State University;* [2]*School of Sustainable Engineering & the Built Environment, Arizona State University*

27 **Photodissociation of Charge Tagged Peptides and Mechanisms for an Unexpected Arginine Effect;** Yi He, Ramakrishnan Parthasarathi, Krishnan Raghavachari, and James P. Reilly; *Department of Chemistry, Indiana University, Bloomington, IN*

28 **Laserspray Ionization, Ion Mobility Spectrometry, and MS/MS: A New Approach for Protein Characterization;** Ellen D. Inutan and Sarah Trimpin; *Wayne State University, Department of Chemistry, Detroit, MI*

29 **Tryptic y^{++} Ion Distributions and Coulombic Repulsion;** Karl K. Irikura[a], John K. Merle[b], and Yamil Simón-Manso[a]; [a] *Chemical and Biochemical Reference Data Division, National Institute of Standards and Technology, Gaithersburg MD;* [b] *Department of Chemistry, Winston-Salem State University, Winston-Salem NC*

30 **High Field Asymmetric Waveform Ion Mobility Spectrometry for Improved Peptide Identification;** Samantha L. Isenberg[1], Alessandra L. Ferzoco[1], Mark E. Ridgeway[2], Desmond A. Kaplan[2], Melvin A. Park[2] and Gary L. Glish[1]; *University of North Carolina, Chapel Hill, NC*[1], *Bruker Daltonics, Billerica, MA*[2]

31 **Characteristics of "a+1" Ions Found in ETD Spectra of Peptides;** Richard S. Johnson, Mike Hoopman, and Robert Moritz; *Institute for Systems Biology, Seattle, WA*

32 **Determining the Size & Charge of Individual Molecules with Single Nanometer-Scale Pores;** John J. Kasianowicz, Joseph W.F. Robertson, & Joseph E. Reiner; *NIST, Physical Measurement Laboratory, Gaithersburg, MD*

33 **Formation of Cyclic Fragment Ions Equivalent to $[y_{n-1} + 10]^+$ in the Collision Induced Dissociation of Protonated Peptide Ions Containing n Amino Acid Residues;** Lisa E. Kilpatrick, Yamil Simón-Manso, Pedatsur Neta, Xiaoyu Yang, and Stephen E. Stein; *NIST, Chemical and Biochemical Reference Data Division, Gaithersburg, MD*

34 **Multiple Fragmentation Approaches for Top-Down Analysis of Ubiquitin: Comparison of CID, ETD, HCD and In-Source Fragmentations;** Min-Sik Kim[1,2], Raghothama Chaerkady[1,4], Robert O'Meally[1,2] and Akhilesh Pandey[1,2,3]; [1]*McKusick-Nathans Institute of Genetic Medicine, Departments of* [2]*Biological Chemistry,* [3]*Oncology and Pathology, Johns Hopkins University School of Medicine, Baltimore MD;* [4]*Institute of Bioinformatics, International Technology Park, Bangalore, Karnataka India*

35 *Promoted poster 15 minute oral presentation during the Sunday Hot Topics II session* - **Investigation of Protein-RNA Cross-Linking by Mass Spectrometry;** Katharina Kramer[1], Petra Hummel[1], He-Hsuan Hsiao[1], Xiao Luo[2], Markus Wahl[2], Henning Urlaub[1]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]Institute for Chemistry and Biochemistry, Freie Universität Berlin, Germany*

36 **Hydrogen Deuterium Exchange Measured at Single-Residue Resolution by Electron Transfer Dissociation High Resolution Mass Spectrometry;** Rachelle R. Landgraf, Michael J. Chalmers, Patrick R. Griffin; *The Scripps Research Institute-Florida, Jupiter, FL*

37 **MS/MS Fragmentation of Cysteine-Modified Peptides Formed via Click Chemistry;** André LeBlanc, Tze Chieh Shiao, Souade Ben Haddou, René Roy, Lekha Sleno*; *Université du Québec à Montréal, Pharmaqam/Chem Dept, Montréal, QC*

38 **Top–Down Fragmentation on a 12T solariX FT-ICR Mass Spectrometer using Precursor Acquisition Independent from Ion Count (PAcIFIC);** CL MacKay[1], A Stokes[1], Y Ting[2], M Karim[1], DR Goodlett[2], P Langridge Smith[1]; *SIRCAMS, School of Chemistry, University of Edinburgh, Edinburgh; Department of Medicinal Chemistry, University of Washington, Seattle, WA*

39 **Protein Profiling of Adenine Nucleotides and Nucleoside Analogues Binding Proteins using Novel Activity Based Protein Profiling Probes;** Shikha Mahajan, David J. Merkler, Roman Manetsch; *Department of Chemistry, University of South Florida, Tampa, Fl*

40 **Implementation of Dual Electrospray Ionization Electron Transfer Dissociation with a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer;** Yuan Mao[a,b], Joshua J. Savory[a], Christopher L. Hendrickson[a,b], Alan G. Marshall[a,b]; *[a] Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [b]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

41 **Enhanced Stable Isotope Analysis using Multiple Orthogonal Separations (UPLC-IMS-MS^{E})** [1]Roy Martin, [1]Michael Nold, [2]Shi-Jian Ding, [1]Scott Geromanos; *[1]Waters Corporation, Beverly MA, [2]Univ. Nebraska Med. Center, Omaha, NE*

42 **Applying Complimentary MS-Based Peptide Sequencing and Label-Free Quantification Strategies for Comprehensive Investigation of Proteome Changes in Undifferentiated hBM-MSCs;** Samuel T. Mindaye, Peter Frank, Michial A. Alterman; *Tumor Vaccines and Biotechnology Branch, Division of Cellular and Gene Therapies, Center for Biologics Evaluation and Research, Food and Drug Administration, Bethesda, MD*

43 **Ehrenfest Dynamics of Electron Based Dissociations;** Christopher Moss, Xiaosong Li, Frantisek Turecek; *Department of Chemistry, University of Washington, Seattle, WA*

44 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Characterising the Behaviour of Lys-N peptides in Tandem Mass Spectrometry;** Shabaz Mohammed, Nadia Taouatas, Paul J. Boersema, Marco L. Hennrich, Nikolai Mischerikow, Maarten Altelaar and Albert J.R. Heck; *Utrecht University, Utrecht, The Netherlands*

45 **Expert System for Automated Annotation of High Resolution MS/MS Spectra;** Nadin Neuhauser, Annette Michalski, Jürgen Cox, Matthias Mann; *Max Planck Institute for Biochemistry, Martinsried, Germany*

46 **Analysis of the Interactome of Modified Chromatin using Quantitative Mass Spectrometry;** Miroslav Nikolov[1], Alexandra Stützer[2], Andrius Krasauskas[3], Kerstin Mosch[2], Szabolcs Soeroes[2], Holger Stark[3], Henning Urlaub[1] and Wolfgang Fischle[2]; *[1] Bioanalytical Mass Spectrometry Group, [2] Laboratory of Chromatin Biochemistry, [3] 3D Electron Cryo-Microscopy Group, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany*

47 **Probing Conformational Changes and Peptide Ion Fragmentation by Multidimensional Ion Mobility Spectrometry–Mass Spectrometry;** Nicholas A. Pierson and David E. Clemmer; *Department of Chemistry, Indiana University, Bloomington, IN*

48 **On the Relevance of Peptide Sequence Permutations in Shot-Gun Proteomics Studies;** Long Yu,[1] Yanglan Tan,[1] Yihsuan Tsai,[2] David R. Goodlett,[2] and Nick C. Polfer[1]; [1] *Department of Chemistry, University of Florida, Gainesville, FL;* [2] *Department of Medicinal Chemistry, University of Washington, Seattle, WA*

49 **A Statistical Solution for Pair-Wise Comparative Proteome Analysis using Large Scale Label-Free Spectral Counting;** Anton Poliakov[a], Lalit Ponnala[b], Paul Dominic Olinares[a], Yukari Asakura[a] and Klaas van Wijk[a]; [a]*Department of Plant Biology, Cornell University, Ithaca, NY;* [b]*Computational Biology Service Unit, Cornell University, Ithaca, NY*

50 **Characterization of Gelsolin-Fibronectin Interaction by MALDI-TOF/TOF Mass Spectrometry;** G. Pottiez and P. Ciborowski; *Department of Pharmacology and Experimental Neuroscience, University of Nebraska Medical Center, Omaha, NE*

51 **Dipolar DC Potentials Applied to the End-Cap Electrodes of a 3-D Ion Trap for Collision Induced Dissociation;** Boone M. Prentice[1], Robert E. Santini[2], and Scott A. McLuckey[1]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN;* [2]*The Jonathan Amy Facility for Chemical Instrumentation, Department of Chemistry, Purdue University, West Lafayette, IN*

52 **CID Fragmentation of Bilirubin and its Metabolites;** Kevin Quinn, Troy Wood; *University at Buffalo*

53 **Peptide *de novo* Sequencing by Exploiting High-Energy Fragment Ions;** Xiaohui Liu, Youyou Yang, and James P. Reilly; *Indiana University, Bloomington, IN*

54 **Peptoid Fragmentation under Tandem Mass Spectrometry Conditions;** Kiran Morishetti[1], Xiaoning Zhao[1], Scott Russell[2], Dave Robinson[3] and Jianhua Ren[1*]; [1]*University of the Pacific;* [2]*Cal State Stanislaus;* [3]*Sandia National Laboratory*

55 **Sequencing Clustered *O*-glycopeptides by Use of ECT/ETD Fragmentation and Overlapping Proteolytic Fragments;** Kazuo Takahashi, Archer D. Smith, IV, Jan Novak, and Matthew B. Renfrow; *Biomedical FT-ICR MS Laboratory, Departments of Biochemistry and Microbiology, University of Alabama, Birmingham, AL*

56 **Structural Characterization of Peptides and Proteins Directly from Mouse Brain Tissue using Laserspray Ionization Mass Spectrometry;** Alicia Richards and Sarah Trimpin; *Wayne State University, Detroit, MI*

57 **Challenges in Identification of the N-Terminal Isoaspartic Acid Residue Probed by Electron Activated Fragmentation Methods;** Nadezda P. Sargaeva[1], Cheng Lin[1], Peter B. O'Connor [1, 2]; [1]*Boston University School of Medicine, Boston, MA;* [2]*University of Warwick, Coventry, UK*

58 **Fundamental Studies of Inter- and Intramolecular Disulfide Bond Cleavages in Model Peptides by Covalently Attached Acetyl Radical;** Chang Ho Sohn, Tae-Young Kim and J. L. Beauchamp*; *Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA*

59 *Promoted poster 15 minute oral presentation during the Sunday Hot Topics II session* - **Factors Influencing Neuropeptide Identification in a Database Search;** Bruce Southey[1], Kyuil Cho[1], Jonathan Sweedler[2] and Sandra Rodriguez Zas[1]; [1]*Department of Animal Sciences, University of Illinois at Urbana Champaign;* [2]*Department of Chemistry, University of Illinois at Urbana Champaign*

60 **Integration of Bioinformatics and Empirical Resources for Neuropeptide Identification;** Bruce Southey[1], Maria Fälth[2], Per Andrén[2], Jonathan Sweedler[3] and Sandra Rodriguez Zas[1]; [1]*Department of Animal Sciences, University of Illinois at Urbana Champaign;* [2]*Department of Pharmaceutical Biosciences, Medical Mass Spectrometry, Uppsala University;* [3]*Department of Chemistry, University of Illinois at Urbana Champaign*

61 **From Wheat to *Brachypodium distachyon*: How Does the Application of a Viral Stress Lead to Heritable Protection against Fusarium Head Blight (FHB) in Wheat?** D. Shearer [1], S. Haber [2], V. Spicer [1,3], O. Krokhin [3], M. Harder [1], N. Lovat [1], D.L. Seifers [4], J. Gilbert [2], and K.G. Standing **[**1,3]; *[1] TOFMS Lab, Department of Physics & Astronomy, University of Manitoba; [2] Cereal Research Centre, Agriculture & Agrifood Canada, Winnipeg, Manitoba; [3] Manitoba Centre for Proteomics & Systems Biology, University of Manitoba; [4] Kansas State University*

62 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session -* **Energetics of Protonated Peptide Fragmentation Measured by Threshold Collision-Induced Dissociation;** Michael van Stipdonk[1], Abhigya Mookherjee[2], Samuel P. Molesworth[1], Peter B. Armentrout[2]; [1]*Department of Chemistry, Wichita State University, Wichita KS;* [2]*Department of Chemistry, University of Utah, Salt Lake City UT*

63 *Promoted poster 15 minute oral presentation during the Sunday Vendor Workshop session -* **An Unbiased Approach to Increasing Proteome Coverage Using Ion Mobility with MS^E;** Martha Stapels, Keith Fadgen, Scott Geromanos, and Jim Langridge; *Waters Corporation, Milford, MA*

64 **Characterization of Differentiation Factors in Human Non-Pigmented Ciliary Epithelium Cell Secretome;** Raghu R. Krishnamoorthy[1], Yu-Shian Su[2], Shiang-Bin Jong[2], Tze-Wen Chung[3], Yuan-Han Yang[4], Thomas Yorio[1], Ming-Hui Yang[3,*],Yu-Chang Tyan[2,*]; [1] *Department of Pharmacology and Neuroscience, University of North Texas Health Science Center;* [2] *Department of Medical Imaging and Radiological Sciences, Kaohsiung Medical University;* [3] *Department of Chemical and Material Engineering, National Yulin University of Science and Technology;* [4] *Department of Neurology, Kaohsiung Medical University Chung-Ho Memorial Hospital*

65 **High Field Asymmetric Waveform Ion Mobility Spectrometry for Improved Peptide Identification by Tandem Mass Spectrometry;** Swearingen, K.E., Johnson, R.S., and Moritz, R.L.; *Institute for Systems Biology, Seattle, WA*

66 **Disfavoring Macrocycle b Fragments by Constraining Torsional Freedom: The "twisted" ase of QWFGLM b_6;** Marcus Tirado,[a] Xian Chen,[a] Alfred Yeung,[a] Jeffrey D. Steill,[b] Jos Oomens[b] and Nick C. Polfer[a], [a]*Department of Chemistry, University of Florida, Gainesville, FL;* [b]*FOM Institute "Rijnhuizen", Nieuwegein, The Netherlands*

67 **Characterization of Urinary Proteome from Blackfoot Disease Endemic Areas - The Over-Expression of SPINK5, ADAM28 and PTP1 in Bladder Transitional Cell Carcinomas;** Ming-Hui Yang[1], Yu-Chang Tyan[2], Lia-Beng Tan[3], Pao-Chi Liao[3]; [1] *Department of Chemical and Material Engineering, National Yulin University of Science and Technology;* [2] *Department of Medical Imaging and Radiological Sciences, Kaohsiung Medical University;* [3] *Department of Environmental and Occupational Health, National Cheng Kung University*

68 **Negative Ion Electron Capture Dissociation (niECD) of Disulfide-Linked Peptide Anions;** Ning Wang, Kristina Håkansson; *Department of Chemistry, University of Michigan, Ann Arbor, MI*

69 **Ion Trap DC CID: Fundamentals and Applications in a qTOF Instrument;** Ian K. Webb[1], Frank A. Londry[2], Scott A. McLuckey[1]; [1]*Purdue University, Department of Chemistry, West Lafayette, IN;* [2]*AB SCIEX, Concord, Ontario, Canada*

70 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Investigation of Database Search Tools and Parameters for Identification of Endogenous CNS Peptides/Proteins Analyzed by an Online Top-Down MS Approach;** Ann Westman-Brinkmalm, Erik Portelius, Annika Öhrfelt, Rita Persson, Maria Olsson, Mikael Gustavsson, Henrik Zetterberg, Kaj Blennow, and Gunnar Brinkmalm; *Inst. Neuroscience and Physiology, Univ. Gothenburg, Sahlgrenska University Hospital, Mölndal, Sweden*

71 **Analysis of Complex Oligosaccharides from Glycopeptides and Glycoproteins using Multi-Stage Mass Spectrometry and Oligosaccharides Spectral Library;** Fan Xiang; *Shimadzu*

72 **PeaksDB: Substantially Improved Peptide Identification with ETD Mass Spectrometry;** Jing Zhang[1], Lei Xin[1], Paul Shan[1], Bin Ma[2]; [1] *Bioinformatics Solutions Inc.* [2] *University of Waterloo*

73 **Database Search Algorithm for Identification of Cross-Links in Proteins using Tandem Mass Spectrometry;** Hua Xu[1*], Pang-Hung Hsu[2], Ming-Daw Tsai[3,4], Michael A. Freitas[5]; [1]*Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH;* [2]*Institute of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan;* [3]*The Genomics Research Center, Academia Sinica, Nankang, Taipei, Taiwan;* [4]*Institute of Biological Chemistry, Academia Sinica, Nankang, Taipei, Taiwan;* [5]*Department of Molecular Immunology Virology and Medical Genetics, The Ohio State University, Columbus, OH*

74 *Promoted poster 15 minute oral presentation during the Saturday Hot Topics I session* - **Proteome-Wide Detection and Quantification of Isoaspartyl Residues by ETD FTMS;** Hongqian Yang, Yaroslav Lyutvinskiy, David M. Good, and Roman A. Zubarev; *Division of Molecular Biometry, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Stockholm, Sweden*

75 **Proteomics in Alzheimer's Disease: Identification for Alzheimer's Disease-Related Proteins;** Ming-Hui Yang[1], Yu-Chang Tyan[2,*], Yuan-Han Yang[3]; [1] *Department of Chemical and Material Engineering, National Yulin University of Science and Technology;* [2] *Department of Medical Imaging and Radiological Sciences, Kaohsiung Medical University;* [3] *Department of Neurology, Kaohsiung Medical University Chung-Ho Memorial Hospital*

76 **Top-Down Mass Spectrometric Sequencing of Native Peptides in Plasma and CSF for a Peptidomics Database;** Hans-Dieter Zucht[1], Stephan Jung[1], David Britton[2], Malcolm Ward[2], Sasa Koncarevic[1], Karsten Kuhn[1], Marco Schärfke[1], Petra Budde[1]; [1]*Proteome Sciences R&D GmbH Co. KG, Altenhöferallee 3, 60438 Frankfurt am Main, Germany;* [2]*Proteome Sciences plc*

77 *Promoted poster 15 minute oral presentation during the Sunday Hot Topics II session* - **Combining HCD and ETD to Determine Sites of O-GlcNAc Modification;** Peng Zhao[1], Rosa Viner[2], Chin Fen Teo[1], David Horn[2], Lance Wells[1]; [1]*University of Georgia, Complex Carbohydrate Research Center, Athens, GA;* [2]*Thermo Fisher Scientific, San Jose, CA*