

LAKE LOUISE XVI

16th Workshop on Tandem Mass Spectrometry

Thursday, December 4, 2003

Chair: Gary Glish

- 8:05 Introductory Remarks
- 8:15 Copper-Mediated Radical Cations of Peptides, *K.W. Michael Siu*, York U.
- 8:55 Controlling fragmentation of peptides for protein identification, Isabel Riba Garcia, *Simon Gaskell*, UMIST
- 9:15 Peptide Fragmentation as a function of Laser Fluence in a MALDI TOF-TOF, *Alfred Yergey*¹, Jennifer Campbell², Paul Blank¹, Marvin Vestal², Stephan Stein³, ¹NIH, ²ABI, ³NIST
- 9:35 Surface-Induced Dissociation of MALDI Ions in FT-ICR MS, *Julia Laskin*, Kenneth Beck, John Hache, Jean Futrell, PNL

9:55 Discussion

10:00 Break

- 10:20 Linear Quadrupoles with Added Octopole Fields, *Don Douglas*, U. of British Columbia
- 10:40 Using Single Analyte Resolved In-Source CID and Accurate Mass Measurement for the Analysis of Peptides and Small Molecules, *John Fjeldsted*, Agilent
- 11:00 Travelling Wave Ion Propulsion in a Collision Cell, *Kevin Giles*, Steve Pringle, Ken Worthington, Bob Bateman, Waters Corp.
- 11:20 ECD and Positive Ion/Negative Ion Reactions in the IonSpec Closed Cylindrical Cell, *Robert T. McIver*, Kevin Crellin, IonSpec Corp.
- 11:40 High Throughput, Data Dependent Analysis using a Hybrid Ion Trap-FTICR Mass Spectrometer, *Lester Taylor*, Thermo Electron Corp.

12:00 Discussion

Chair: Paul Mayer

- 14:00 Protein Folding Mechanisms and Noncovalent Ligand-Protein Interactions Studied by ESI-MS, *Lars Konermann*, Sonya M. Clark, Douglas A. Simmons, Derek J. Wilson, U. of Western Ontario
- 14:40 A Proteomic Approach for Identification of Bacteria Using Tandem Mass Spectrometry, *Jacek P. Dworzanski*, A. Peter Snyder, Rui Chen, Haiyan Zhang, David Wishart, Liang Li, Geo-Centers, Inc./US Army Edgewood Chemical Biological Center
- 15:00 Direct identification of low mass bacterial biomarkers by MALDI MS and MS/MS of whole cells, *V. Ruelle*¹, P. Verhaert², E. De Pauw¹, ¹U. of Liège, ²U. of Leuven and U. of Maastricht

15:20 Discussion

15:25 Break

- 15:50 Environmental Mass Spectrometry: Emerging Contaminants and Current Issues, *Susan Richardson*, US EPA
- 16:30 A Tandem Mass Spectrometric Study at High Mass Accuracy of Flavonoid Mono- and Di-glycosides, *Raymond E. March*¹, Errol G. Lewars¹, C. Stadey¹, Xiu-Sheng Miao¹, Chris D. Metcalfe¹, Maciej Stobiecki², Lukasz Marczak², ¹Trent U., ²Polish Academy of Science

- 16:50 Offline HPLC - MALDI Tandem Mass Spectrometry for the Quantification of Pharmaceutical Drugs, *Panos Hatsis*, Dietrich A. Volmer, Institute for Marine Biosciences
- 17:10 Even clinicians prefer Tandem MS test results over immunoassays for differential diagnosis of various diseases, *Ravinder J. Singh*, Mayo Clinic

17:30 Discussion
Break for dinner

Chair: Gord McKay

- 20:00 From Milligrams to Femtograms : A Mass Spec Analyst's Experience Through Thirty Years, *Lawrence Hogge* and Colleagues

21:00 Discussion
21:10 Poster Session

Friday, December 5, 2003

Chair: John Klassen

- 8:30 Folding and Dynamics of Proteins and Protein Complexes Monitored by Mass Spectrometry, *Albert Heck*, Utrecht U.
- 9:10 Top Down MS/MS Characterization of Disulfide Bonds by Electron Capture Dissociation and IR Multiphoton Dissociation, *Huili Zhai*, Fred McLafferty, Cornell U.
- 9:30 Initiating Analysis of the Proteome of the Ciliated Protozoan *Tetrahymena thermophila*, *Jeffrey C. Smith*, Kalkidan Belay, Scott Beeser, Alex Keuroghlian, Ronald E. Pearlman, K.W. Michael Siu, York U.
- 9:50 Tissue Proteomics: An Analytical Chemist's Dream (and Nightmare), *Liang Li*, U. Alberta

10:10 Discussion

10:15 Break

- 10:35 Towards Quantifying Internal Energy Deposition at keV Collision Energies, Clement Poon, *Paul M. Mayer*, U. of Ottawa
- 10:55 Spin Conservation in the Unimolecular Dissociation of Ionic Complexes between NO and Aromatics, *Julie A.D. Grabow*, Paul M. Mayer, U. of Ottawa
- 11:15 Comparative Analysis of Peptide Modifications on Quadrupole-Linear Ion Trap and Quadrupole-Time of flight Instruments, *Juergen Kast*, U. of British Columbia
- 11:35 Imaging MALDI with an orthogonal TOF mass spectrometer, *Werner Ens*, Gamini Piyadasa, James McNabb, Victor Spicer, Kenneth G Standing, U. of Manitoba

11:55 Discussion
Afternoon Free

19:00 Workshop Banquet

Saturday, December 6, 2003

Chair: Simon Gaskell

- 8:45 Isotopically Coded Cleavable Crosslinker Combined with Tandem MS for Studying Protein Complexes, *Christoph Borchers*, U. of North Carolina
- 9:05 Structural Characterisation of Outer Cell-Envelope Glycoproteins and their Glycans from *Mycobacterium avium*, *A.M. Taylor*¹, A. Gruhl², O. Holst², J.E. Thomas-Oates¹, ¹U. of York, ² Borstel Research Centre

9:25 A Novel Approach for Mapping O-Linked Glycosylation in *Pseudomonas Aeruginosa* Through Comparison of Isotope Maps Before and After β -Elimination Followed by Targeted LC/MS/MS, **Michael Schirm**¹; Susan Logan²; I. Schoenhofen²; Karen Waldron¹; Pierre Thibault³, ¹U. of Montreal, ²Institute for Biological Sciences, ³Caprion Pharmaceuticals Inc

9:45 Discussion

9:55 Break

10:15 Techniques for Enhanced High-Throughput HPLC/MALDI-MS/MS Analysis of Small Pharmaceutical Drugs, **Dietrich Volmer**, Institute for Marine Biosciences

10:35 Determinations of Protein Complex Association Constants with the Titration Method: Constraints Imposed by the ESI Mechanism, Michael Peschke, Udo Verkerk, **Paul Kebarle**, U. Alberta

10:55 How much mass accuracy is needed for high throughput proteomics, **Daniel Boismenu**, McGill U.

11:15 Direct tissue peptidomics; evolution in the past two years, **Peter Verhaert**, U. of Leuven and U. of Maastricht

11:35 IRMPD of Intact Proteins in a Quadrupole Ion Trap, David M. Black, Johanna Stephens, **Gary L. Glish**, U. of North Carolina

11:55 Closing Remarks

Posters

Analysis of cisplatin and its hydrolysis products by ESI-ITMS and high-field asymmetric waveform ion mobility spectrometry, Meng Cui, Luyi Ding and **Zoltán Mester**, Institute for National Measurement Standards, National Research Council Canada

How to not re-sequence a proteome: Peptide MS/MS Libraries, **Wade Hines**, Beyond Genomics

Comparative Proteomics by Isotopic Coding of Lysine Residues, **Jeremy E. Melanson**, Kenneth A. Chisholm, Steven J. Locke, Devanand M. Pinto, Institute for Marine Biosciences

Approaches to the analysis of 3-chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone (MX) : a mass spectrometric study, M.A. Trikoupis, V.Y. Taguchi, Ontario Ministry of the Environment
Recent Experiences with a QToF Instrument for the Analysis of Chemical Warfare Agents, **Paul A. D'Agostino**, **Claude L. Chenier**, James R. Hancock, DRDC

Two Dimensional Offline HPLC/MS/MS as a tool to elucidate differences in Protein Expression patterns from patients with a genetic disorder and their healthy relatives, Martin Vollmer¹, Patric Hörth¹, Edgar Nägele¹, **Linda Côté**¹ Friedhelm Hildebrandt², ¹Agilent, ²U. of Michigan

Laser Desorption, Uv-Resonant Multiphoton Ionization, And Tunable Resonant Photodissociation Of Large Molecules In Ion-Trap MS, Mike Blades, August Specht, Denis Roland, John Hepburn, Ken Wright, U. of British Columbia

Fluorescence Spectroscopy of Molecular Ions in a Paul Trap, **Mike Blades**, Ken Wright, U. of British Columbia

Detection of Phosphorylated Peptides from Data Dependent MS3 Neutral-Loss Scans using a Linear Ion Trap Mass Spectrometer, Amy Zumwalt, Gargi Choudhary, Diane Cho, Eric Hemenway, Iain Mylchreest, Thermo Electron Corp.

Shotgun Sequencing of the Human Cerebrospinal Fluid Proteome Using 2D Chromatography in Combination with Linear Ion Trap Mass Spectrometry, A.F. Hühmer¹, R.G. Biringer¹, H. Amato¹, M. Harrington², ¹Thermo Electron, ²Huntington Research Institutes

Quantification of Selected Sulfonylurea Herbicides in Canadian Prairie Wetlands Utilizing Electrospray Ionization Mass Spectrometry and Multiple Reaction Monitoring, John V. Headley, *Kerry M. Peru*, Allan Cessna, Jonathan Bailey, Environment Canada

A Preliminary Comparison of MASCOT, MASCOT Distiller and ProteinLynx Global Server 2.0 for Searching Primary Sequence Databases using Peptide LC-MS/MS Data, *Doug Olson*, Andrew Ross, NRC Saskatoon

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