

LAKE LOUISE XVII

17th Workshop on Tandem Mass Spectrometry

Thursday, December 2, 2004

Chair: *Paul Mayer*

- 8:05 Introductory Remarks, Gary Glish
- 8:15 Tandem Mass Spectrometry and Proteomics in the Search for the Antigenic Peptide that Causes Type I Diabetes, *Michael L. Gross*, E. R. Unanue, J. Walters, A. Suri, I. Vidavsky, Washington University
- 8:55 Bottom-up and Top-down Proteomics for Comprehensive Protein Characterization, *Christoph Borchers*, U. North Carolina
- 9:15 Profiling Protein Localization and Interactions with GFP-Tagged Proteins, *Ileana M. Cristea*, Brian T. Chait, Michael P. Rout, Rockefeller U
- 9:35 Dissociation of Multiprotein Complexes in the Gas Phase. Influence of Coulombic Repulsion on Pathways and Energetics, Igor Sinelnikov, Elena Kitova, *John S. Klassen*, U. Alberta
- 9:55 Discussion**
- 10:00 Break**
- 10:20 Unambiguous Assignment of Intra-Molecular Chemical Cross-Links in Modified Mammalian Membrane Proteins by Fourier Transform-Tandem Mass Spectrometry, G. *H. Kruppa*^{1,3}, P. Novak¹, W. E. Haskins^{1,2}, M. D. Leavell¹, M. J. Ayson¹, R. B. Jacobsen¹, J. S. Schoeniger¹, M. M. Young¹, ¹Sandia National Laboratory, ²Genentech, ³Bruker Daltonics
- 10:40 Unfolding and Subunit Disassembly of Large Noncovalent Protein Complexes Studied by Time-Resolved ESI-MS, *Lars Konermann*, Douglas A. Simmons, Derek J. Wilson, University of Western Ontario
- 11:00 Recent Development of LC-MALDI MS and MS/MS for Proteomics, *Liang Li*, U. Alberta
- 11:20 Tandem Mass Spectrometric Approaches to the Analysis of the African Trypanosomal Flagellar Proteome, *Sarah Hart*, Simon Gaskell, U. Manchester
- 11:40 Ion-Ion And Ion-Molecule Reactions on the Surface of Proteins Produced by Nanospray, Udo H. Verkerk, *Paul Kebarle*, U. Alberta
- 12:00 Discussion**

Chair *Gord McKay*

- 14:00 PEPICO Studies of Competitive and Sequential Ionic Reactions, *Tomas Baer*¹, Balint Sztaray², ¹U. North Carolina, ²Eotvos Lorand U.
- 14:40 TPEPICO Rate Constants From Variable Extraction Delay Experiments at the Daresbury Synchrotron, *Paul Mayer*¹, Emma E. Rennie¹, Anne-Marie Boulanger¹, David M. P. Holland², David A. Shaw², Louise Cooper³, Christopher A. F. Johnson³, John E. Parker³, ¹U. Ottawa, ²Daresbury Laboratory, ³Heriot-Watt U.
- 15:00 Generation and Reactions of Anionic s-Adducts of 1,3-Dinitrobenzene, 1,3,5-Trinitrobenzene and halonitrobenzenes with Carbanions in a Gas Phase, *Tomasz Bienkowski*, Witold Danikiewicz and Dorota Kozowska, Polish Academy of Sciences
- 15:20 Mechanism of the Isomerization of Acetaldehyde Ion into the Vinyl Alcohol Ion, *Xian Wang*, John Holmes, U. Ottawa

15:40 Discussion

15:45 Break

16:10 Managing Accuracy, Precision, AND High Sample Workloads with LC/MS/MS in the Regulated CRO Environment, *Ronald E. Shoup*, Bioanalytical Systems Inc.

16:50 A Novel Qualitative and Quantitative LC-MS Based Approach to Protein Profiling and Biomarker Discovery, *Mark A. McDowall*, Scott Geromanos, Keith Richardson, Phillip Young, Richard Denny, Kieran Neeson, Therese McKenna, Craig Doerschel, Marc Gorenstein, Guo-Zhong Li, Timothy Riley, Jeffrey C. Silva, Jim Langridge, Waters Corporation

17:10 Profiling Phytohormones and their Metabolites by LC-MS/MS, *Andrew Ross*, Steve Ambrose, Sheila Chiwocha, Allan Feurtado, Ken Nelson, Sue Abrams, NRC

17:30 Discussion

Chair Orval Mamer

20:00 Mass Spectral Analysis of the Reactions of Thiols with Angeli's Salt, *Biao Shen*, A. M. English, Concordia U.

20:20 TOMAS: Toolbox for Mass Spectrometry Data Analysis, *Frank R. Morales*, Robert Kearney, Zsuzsanna Benesath-Makkai, Daniel Boismenu, Elie Na, McGill University

20:40 Enabling Technologies at the Limit of Detection, *Ken K.-C. Yeung*, Haixia Zhang, Chandra Nesbitt, U. Western Ontario

21:00 Discussion

21:05 Poster Session

Mass Analysis of Polypeptide Ladders Generated from Microwave-Assisted Acid Hydrolysis of Proteins: A New Tool for Protein Sequencing and Analysis of Protein Modifications, *Hongying Zhong*, Liang Li, U. Alberta

Global Quantitative Profiling of Protein Mixtures Using Differential Stable Isotopic Labeling and Microbore LC MALDI QqTOF MS, *Chengjie Ji*, Liang Li, U. Alberta

Determination of Imidacloprid in Environmental Samples by LC-MS/MS, *Kerry Peru*, Jonathan Bailey, John Headley, Allan Cessna, Environment Canada

Simulation of High-Resolving Quadrupoles with Collisional Cooling Interface and Fringing Fields, *Michael Sudakov*, Shimadzu Research Laboratory

Exploring Hydrogen/Deuterium Scrambling Through Tandem MS of Specifically Engineered Peptides, *John Chik*, David C. Schriemer, U. Calgary

Nano-electrospray-LC/MS/MS using a Polymer Microfluidic Device for Protein Identification, *Linda Côté*, Kevin Killeen, Hongfeng Yin, Georges L. Gauthier, Karsten Kraiczek, Agilent Technologies

Comparison of Solution Phase Isoelectric Focusing and Ion Exchange Chromatography for Intact Protein Fractionation in a Novel LC/MS/MS Strategy, John Tran¹, Chelsea Thorne¹, Devanand Pinto², *Alan Doucette*², ¹Dalhousie U. ²NRC Institute for Marine Biosciences

Ion/Ion Reactions in a Hybrid Linear Ion Trap Tandem Mass Spectrometer, *Jin Wu*¹ Yu Xia², James W. Hager³, Frank A. Londry³, Scott A. McLuckey², ¹Merck Frosst, ²Purdue U., ³MDS SCIEX

Blending Antibodies and Sequence Tags for Biomarker Tracking, *Nicola E. Burdeniuk*, David C. Schriemer, U. Calgary

N-Linked Carbohydrate Analysis of IEF-Separated Recombinant Human Gonadotropin Isoforms by Nanospray Q-TOF MS/MS, *Stefan Clerens*, Peter Verhaert, Lutgarde Arckens, U. Leuven

The Decarbonylation of the Acetamide Radical Cation and the Enolization of Its Dimer by Self Catalysis, *M.A. Trikoupis*, P.C. Burgers, P.J.A. Ruttink, J.K. Terlouw, Ontario Ministry of the Environment

Identification of Polyaromatic Sulfur Heterocycles Using Post Column Addition of Tropylium and Tandem Mass Spectrometry, *Walter E. Rudzinski*, Vidja Rai, Texas State U.

Progress Towards Routine Top-Down Primary Structure Determination of Intact Proteins by MALDI-TOF Metastable Ion In-Source Decay Analysis, W. Chen, J. Haddow, *R.W. Olafson*, U. Victoria

High Resolution LC-MS/MS Analysis of Sample Extracts Containing Chemical Warfare Agents, *Paul A. D'Agostino*, Claude L. Chenier, James R. Hancock, DRDC Suffield

Identification of Bacterial and Archaeal Lipids Such as Phospholipids and Archaeols, Using LC-MS (Ion Trap) Techniques, *Thomas Oldenburg*, Kim Noke, Steve Larter, U. Calgary

Toxicology Drug Screening by CE-MSⁿ - a Preliminary Case Example, Doug Knisley, Mark Hetherington, *Gordon McKay*, Pharmalytics Inc, U.Saskatchewan

Screening for Beta-lactam Antibiotics in Milk using Selected Reaction Monitoring MS, *D. A. Durden* and J. Wang, Canadian Food Inspection Agency, Calgary

Amino Acid Determination by FAIMS MS, Margaret McCooye and *Zoltan Mester*, National Research Council

Friday, December 3, 2004

Chair Simon Gaskell

8:15 Characterization of Oligonucleotides by High Performance Tandem MS - Applications in the Biotech Arena, *Steven Hofstadler*, Isis Pharmaceuticals

8:55 Towards Automated Mass Spectrometric Proteome Mining From Unannotated Genomic Information: A Robust Analysis of the *Tetrahymena Thermophila* Axoneme, *Jeffrey C. Smith*¹ Jyoti Garg¹, Julian G.B. Northey², Ronald E. Pearlman¹, K. W. Michael Siu¹, ¹York U., ²U. Toronto

9:15 The Discovery, Identification and Verification of Endometrial Cancer Markers, Leroi DeSouza¹, Jingzhong Guo¹, Mary Joe Rodrigues², Alexander D. Romaschin^{3,4}, Terence J. Colgan^{2,4}, *K.W. Michael Siu*¹, ¹York U., ²Mount Sinai Hospital, ³Toronto General Hospital, ⁴U. Toronto

9:35 Elucidation of the Molecular Structure of Lipid A Isolated From a Rough Mutant Lipopolysaccharide *Aeromonas Salmonicida* Using Electrospray Ionization Quadrupole

Time-Of-Flight Tandem Mass Spectrometry, *Anas El-Aneel*¹, Joseph H. Banoub²,
¹Memorial U., ²Fisheries and Oceans Canada

9:55 Discussion

10:00 Break

10:20 Tandem Mass Spectrometry Studies on Disinfection By-Products, *M.A. Trikoupis*, V.Y. Taguchi, Ontario Ministry of the Environment

10:40 Identification of Multiple C-terminal Peptides of the *Porphyromonas gingivialis* Carboxypeptidase CPG70 and Cysteine Proteinase RgpB Using NanoLC-Ion Trap Mass Spectrometry, *Yu-Yen Chen*, Dina Chen, Paul Veith, Eric Reynolds, U. Melbourne

11:00 Automated Chip-Based Nanoelectrospray Mass Spectrometry for Protein Identification and Characterization, *Colleen K. Van Pelt*, Sheng Zhang, Advion BioSciences

11:20 Porous Polymer Assisted Nanospray, Terry Koerner, Laurie Brown, Stephen Lee, Kiera Turck, *Richard D. Oleschuk*, Queens U

11:40 Factors Affecting Breakdown of S-nitrosothiols in a Z-spray ESI source, *E. E. Moran*, A. M. English, Concordia U

12:00 Discussion

Afternoon Free

Saturday, December 4, 2004

Chair John Klassen

8:45 MSⁿ on a QqTOF System: Dissociative Ping Pong, *Bruce Thomson*, Igor Chernushevich, MDS Sciex

9:25 Fragmentation of Leucine Enkephalin as a Function of Laser Fluence in a MALDI TOF-TOF, *Alfred Yergey*, NIH

9:45 Derivatization for Peptide Characterisation: Is it Worth the Trouble?, *Simon Gaskell*, U. Manchester

9:55 Discussion

10:15 Break

10:35 Another Year of Direct Tissue Neuropeptide MS and Tandem MS Analysis: Progress and Perspectives, *Peter Verhaert*, Stefan Clerens, Babs Van de Plas, Lutgarde Arckens, U. Leuven

10:55 Assistance in Protein Identification by HPLC-MALDI MS/MS Using Peptide Retention Times Prediction, *O. Krokhin*, S. Ying, V. Spicer, W. Ens, J. Wilkins, K. Standing, University of Manitoba

11:15 Ion Excitation in a Linear Quadrupole Ion Trap with Added Octopole Field, Anthony Michaud, Chuanfan Ding, Aaron Frank, Xianzhen Zhao and *Don Douglas*, U. British Columbia

11:35 AP and Vacuum MALDI on a QqLIT Instrument, *Brad Schneider*, Chris Lock, and Tom Covey, Sciex

11:55 The Structure of b_n Ions?, Julia Allen, Phillip Remes, Dave Black, *Gary Glish*, U. North Carolina

Discussion

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