

LAKE LOUISE XXI

21ST Workshop on Tandem Mass Spectrometry

Thursday, December 4, 2008, Morning Session

Chair: Gary Glish

- 8:20 Introductory Remarks: **Gordon McKay**
- 8:25 Gas phase characterization and reactivity of organic ions: experimental and theoretical approaches, **Gianluca Giorgi**, Department of Chemistry, University of Siena, Italy.
- 9:10 Influence of configurational entropy on the dissociation kinetics of protein-ligand complexes in the gas phase, **John Klassen** & Elena Kitova, University of Alberta.
- 9:30 Deuterium scrambling enables high spectral capacity measurements in H/CX-MS Applications, **Dave Schriemer**, Andrew J. Percy, Gordon Slys, C. J. Baher, University of Calgary.

9:50 Discussion

10:00 Break

- 10:20 **Lossing Award Presentation:** Happiness is a magnetic sector mass spectrometer, **Paul M. Mayer**, Chemistry Department, University of Ottawa.
- 11:05 Multi-structured fibers for separation and nanoelectrospray applications, **Richard Oleschuk**, Queens University.
- 11:25 Ion activation for improvement of electron capture dissociation in a linear ion trap, **Jared Bushey**¹, T. Green¹, T. Baba^{1,2}, G. L. Glish¹, ¹University of North Carolina ²Central Research Laboratory, Hitachi Ltd., Tokyo.
- 11:45 Gas phase hemoglobin, J. Wright & **Don Douglas**, Department of Chemistry, The University of British Columbia.
- 12:05 TBA, **Gary Glish**, University of North Carolina.

12:25 Discussion

12:30 Lunch

Afternoon Session

Chair: Susan Richardson

- 14:00 Do iodine contrast media compounds used for medical imaging contribute to the formation of iodinated disinfection by-products in drinking water?, **Susan Richardson**, S. Duirk, C. Lindell, T. Ternes, U. S. EPA, National Exposure Research Laboratory, Athens, GA.
- 14:20 Identification of oxidation products and transformation products of micropollutants: application of liquid chromatography with hybrid triple quadrupole/linear ion trap mass spectrometry, **Jennifer Kormos**, J. Benner, M. Schulz, T. Ternes, Federal Institute of Hydrology (BfG).
- 14:40 On-line large-volume sampling followed by isomer-specific determination of estrogens and their conjugates in water and wastewater samples, **Mehran Alaei**¹, T. Sakuma², S. Caganpan¹, D. Fernandes², R. Ellis², C. Campbell³, M. Takahashi³, B. Wittrig⁴ & R. Lake⁴, ¹Environment Canada, ²Applied Biosystems/MDS Analytical Technologies, ³Shimadzu Scientific Instruments, Inc., ⁴Restek Corporation.

15:00 LC/MS/MS profiling of estrogen metabolism in breast cancer patients to occurrence in water, F. Qin, W. Zhou, J. Boyd, S. Hrudey & *Xing-Fang Li*, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and pathology, Faculty of Medicine and Dentistry, University of Alberta.

15:20 Discussion

15:30 Break

Chair: Lars Konermann

15:50 Chemical strategies for “Targeted” proteome analysis, *Gavin Reid*^{1,2}, A. M. Palumbo¹, J. M. Froelich¹ & Y. Lu¹, ¹Department of Chemistry and ²Department of Biochemistry, Michigan State University.

16:35 Tandem mass spectrometry of biologically active peptides. The amphibian skin peptidome as an ideal model system, *Peter Verhaert*, G. Evaristo-Caprini, M. Pinkse, T. Chen & C. Shaw, Delft University.

16:55 The identification and characterization of the target proteins of R-lacosamide drug, *Onrapak Reamtong*¹, C. E. Evers,² S. W. Cotten², K. D. Park² R. Liu², H. Kohn², S. J. Gaskell¹, ¹The University of Manchester, ²University of North Carolina.

17:15 Protein folding studied by hydrogen exchange, covalent labelling and tandem, mass spectrometry, *Lars Konermann*, Y. Pan, J. Pan, & B. B. Stocks, The University of Western Ontario.

17:35 Discussion

18:00 Dinner

Evening Session

Chair: Orval Mamer

20:00 Characterization of deprotonated trinucleotide and its sodium complex, *Janna Anichina*, E. Jggerud & D. K. Bohme, York University.

20:20 Structures of hydrated LI⁺-Uracil complexes by IRMPD spectroscopy in the N-N/O-H stretching region, *Elizabeth Gillis*, K. Rajabi & T. D. Fidgen, University of Newfoundland.

20:40 Discussion

20:45 Poster Session – please man posters until 23:00

Enhancing the detectability of cysteine-containing peptides, J. M. Bruno¹, N. N. Dicheva², *Carol Parker*², J. C. Edwards¹, ¹Department of Medicine, UNC-Chapel Hill, ²UNC-Duke Proteomics Center, University of North Carolina, Chapel Hill, NC.

Tandem mass spectrometric analysis of novel Gemini surfactant nanoparticles, *Joshua Buse*¹, I. Badea¹, R. E. Verrall² & A. El-Aneed¹, ¹College of Pharmacy and Nutrition, University of Saskatchewan, ²Department of Chemistry, University of Saskatchewan

Rapid analysis of chemical warfare agents by desorption electrospray ionization tandem mass spectrometry, *Paul A. D’Agostino & Claude L. Chenier*, DRDC Suffield.

UPLC-ESI-MS/MS vs. TOF-MS vs. Q-TOF-MS (TOF mode only) for the investigation of wildlife poisoning and the analysis of pesticides in food, **George Keenan**, M. J. Taylor, K. B. Reid & D. U. Fernandez, Science and Advice for Scottish Agriculture, Waters, U. K.

Phosphoproteomic analysis of host signalling events induced by *Salmonella*, **Lindsay D. Rogers**, Y. Fang, E. C. Boyle & L. J. Foster, Department of Biochemistry & molecular Biology and Centre for High-throughput Biology, University of British Columbia.

Site specific analysis of deuterium scrambling, **Tamanna Rob**, L. Lusia & Derek Wilson, ?

Chromatographic calibration in LC-MS analysis: peptide retention standards and universal hydrophobicity, V. Spicer, M. Harder & **Oleg Krokhin**, Manitoba Centre for Proteomics and Systems Biology, University of Manitoba.

LC-MS/MS analysis of imidazolinone herbicides, , A. J. Cessna, **Kerry M. Peru**, **John V. Headley** & Jon Bailey, Environment Canada.

Application of triple quadrupole and quadrupole time of flight tandem mass spectrometry in determination of perfluorooctane sulfonate (PFOS): Identification of interference, fractionation and bioaccumulation of isomers in a Lake Ontario food web, **Mehran Alaei**¹, J. Small¹, M. Houde¹, G. Czub², S. Backus¹, X. Wang¹ & D. Muir¹, ¹Water Science and Technology Directorate, Environment Canada, Department of Applied environmental Science (ITM), Stockholm University.

LC/MS multivariate analysis of beer and targeted MS/MS for the discovery of commercially important compounds, **Linda Côté**¹, M. Maeda², H. Uchida², S. araki², T. Oshima³, Y. Tsuchiya³, K. Maeda³, J. Watari³, S. Fischer⁴, ¹Agilent Technologies Canada Inc, Montréal, ²Agilent Technologies Tokyo, Japan, ³Sapporo Breweries Ltd, Shizuoka, Japan, ⁴Agilent Technologies, Santa Clara, CA.

Combining direct infusion- and LC-MS for comprehensive plant metabolomics, , **Jun Han**¹, R. Danell², D. Lippert², M. Elliott¹, J. Bohlmann³ & Christoph H. Borchers¹, ¹Uvic-Genome BC Proteomics Centre, Victoria, BC, ²Danell Consulting Inc., NC, ³Michael Smith Laboratory, University of British Columbia.

ICC-CLASS: isotopically-coded cleavable cross-linking analysis software suite, **Evgeniy V. Petrotchenko**, & C. H. Borchers, Uvic-Genome BC Proteomics Centre, Victoria, BC.

Development and application of an immuo-MALDI (iMALDI) mass spectrometry assay for diagnosis of hypertension, **Jennifer D. Reid**, D. Holmes & C. H. Borchers, Uvic-Genome BC Proteomics Centre, Victoria, BC.

Imaldi⁺: a targeted proteomics approach to clinical diagnostics, **Brinda Shah**, J. D. Reid & C. H. Borchers, Uvic-Genome BC Proteomics Centre, Victoria, BC.

MRM based, multiplexed, absolute quantitation of 45 proteins in human plasma, **Michael A. Kuzyk**, D. Smith, J. Yang, T. Cross, A. Jackson, d. Hardie, N. L. Anderson & C. H. Borchers, Uvic-Genome BC Proteomics Centre, Victoria, BC.

Benefits of H/D scrambling in bottom-up H/D exchange-MS/MS data analysis, **Andrew J. Percy**, G. W. Slysyz & David Schriemer, University of Calgary.

LC/MS/MS characterization of new nitrosamines in drinking water, **Jessica Boyd**, F. Qin, W. Zhou, Y. Zhao & Xing-Fang Li, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and pathology, faculty of Medicine and Dentistry, University of Alberta..

Comparison between UPLC vs. HPLC tandem mass spectrometry used for quantification in plant hormone profiling, S. Owen, M. Lafond, V. Cekic, D. Van **Steve Ambrose**, I. Zaharia & S. Abrams, NRC Saskatoon.

Friday, Dec. 5, Morning Session

Chair: Gordon McKay

8:20 Evolving MS Technologies and changing workflows in drug metabolism, **Kevin Bateman**, Merck Frosst Canada.

9:05 The expanding role of quantitative LC/MS-based bioanalysis in drug discovery, **Tim Olah**, Bristol Myers Squibb.

9:45 Quantification of therapeutic proteins in human plasma: towards a widely applicable methodology, **Jean-Marie Schmitter**, F. Xuereb, S. Chaignepain, F. Godde, D. Breilh, M. C. Saux, C. Lenz & M. Glueckmann, Institut Européen de Chimie et Biologie (IECB).

10:05 Discussion

10:15 Break

10:35 MS/MS considerations when going from biomarker discovery to biomarker validation, **Christine Miller**, K. Waddell & N. Tang, Agilent Technologies.

10:55 Virtual quantification of metabolites in electrospray ionization-mass spectrometry without chemical standards for metabolomics research, K. Chalcraft, R. Lee & **Philip Britz-McKibbin**, McMaster University.

11:15 Quantitative profiling of secretome during muscle cell differentiation, **Xavia Chan**, S. Ghanny, J. C. McDermott & K. W. M. Siu, York University.

11:35 TMT tandem mass tags, different applications in quantitative proteomics and neurobiology, M.T. Olson, J.A. Epstein, **Martijn Pinkse**, P. Shulz-Knappe & P. Verhaert, Delft University.

11:55 Wheat proteins by new method of plant breeding: their quantitation by tryptic digestion, Itraq, 2TRAQ, 2D-HPLC and TOFMS, K. Haber¹, L. Krokin², V. Spicer^{2,3}, M. Harder³, N. Lovat³ & **Ken Standing**^{2,3}, ¹Cereal Research Centre, Agriculture Canada, ²Manitoba Proteomics Centre, University of Manitoba, ²Department of Physics & Astronomy, University of Manitoba.

12:15 Discussion

12:30 Lunch

14:00 Information walk, with Bob Davidson, up lake (no paddle)

- 16:30** **Broomball: Canada vs. The World**
18:30 **Banquet – Mount Temple Ballroom A**

Sat., Dec. 6, Morning Session

Chair: Orval Mamer

- 8:20 Recent advances in Qtrap technology, **Bruce A. Collings**, M. Guna, T. Biesenthal & M. A. Romaschin, MDS Analytical Technologies.
- 8:40 Atomic weights of the elements: is there anything left for research **Juris Meija**, & Zoltan Mester, National Research Council Canada.
- 9:00 High resolution MS for screening and quantitation applications, **Lester Taylor**, Thermo Fisher Scientific.
- 9:20 “iMALDI”; A targeted approach to clinical diagnostics, **Brinda Shah**, J. D. Reid & C. H. Borchers, Protein Centre, University of Victoria.
- 9:40** **Discussion**
- 9:50** **Break**
- 10:10 Technical characteristics of a new UHR ESI Q-Tof, Ma Xis, **Mike McDonell**, Bruker Daltonics.
- 10:30 Large scale proteome analysis: from identification to quantification, **Liang Li**, University of Alberta.
- 10:50 Structure of radical cation ions in the gas-phase: canonical versus alpha-radical ions, J. Zhao, C.-K. Siu, U. H. Verkerk, A. C. Hopkinson & **Michael Siu**, York University.
- 11:10 A comparison of the performance attributes of optimized DDA versus MSe data acquisition methods for protein identification, **Terry Cyr**, L. Walrond & M. Cameron, Health Canada.
- 11:30 Novel crosslinking reagents and approaches for structural proteomics, **Christoph H. Borchers**, E.V. Petrotchenko, & J. M. Thomas, Protein Centre, University of Victoria.
- 11:50 ?, ?, ?, , Varian.
- 12:10** **Discussion**
- 12:30** **Adjourn and Lunch**