

# LAKE LOUISE XX

## 20<sup>th</sup> Workshop on Tandem Mass Spectrometry

Thursday, November 29, 2007, Morning Session

Chair: *Susan Richardson*

- 8:20 Introductory Remarks: **Gordon McKay**
- 8:25 Tandem mass spectrometry: the key technique for discovering the presence of pharmaceuticals in the environment, **Thomas Ternes**, D. Löffler, M. Schulz, M. Schluesener, Federal Institute of Hydrology, Germany.
- 9:10 Determination of steroids in water, biosolids, and tissues by derivatization GC/MS/MS with isotopic dilution, **James L. Gray**, W.T. Foreman, C.E. Lindley, M.R. Burkhardt, L.B. Barber, US Geological Survey.
- 9:40 LC-MS-MS characterization of trace nitrosamines and arsenics in drinking water and studies of protein interactions, **XingFang Li**<sup>1</sup>, Yuanyuan Zhao<sup>1</sup>, J. Boyd<sup>1</sup>, M. Wagner<sup>1</sup>, C. Le<sup>1</sup>, Meiling Lu<sup>1</sup>, S. Richardson<sup>2</sup>, <sup>1</sup>University of Alberta, <sup>2</sup>US Environmental Protection Agency.

**10:10 Discussion**

**10:15 Break**

- 10:35 Effects of oxidation on the folding and assembly of hemoglobin, **Brian L. Boys**, M.C. Kuprowski and L. Konermann, University of Western Ontario.
- 10:55 Tandem mass spectrometry of arsenic interactions with hemoglobin and the consequent health implications, **Chris Le**, University of Alberta.
- 11:15 Characterization of the fate of complex naphthenic acid mixtures by capillary HPLC/QTOF-MS, **Xiumei Han**<sup>1</sup>, K.M. Peru<sup>2</sup>, J.V. Headley<sup>2</sup>, J.W. Martin<sup>1</sup>, <sup>1</sup>University of Alberta, <sup>2</sup>Environment Canada.
- 11:35 Innovative approaches to meeting the challenges in drinking water analysis with Varian liquid chromatography, triple quadrupole MS/MS technology, **Marcus Kim**<sup>1</sup>, E. George<sup>2</sup>, T Payne<sup>2</sup>, <sup>1</sup>Varian Canada Inc, <sup>2</sup>Walnut Creek, CA.
- 11:55 The identification of influenza strains by tandem MS: it is better to be lucky than good, **Terry Cyr**, D. Bertrand and M. Cameron, Centre for Biologics Research, Tunney's Pasture.

**12:15 Discussion**

**12:30 Lunch**

### Afternoon Session

Chair: *Paul Mayer*

- 14:00 Enhanced information from ambient ionisation experiments, **Jim Scrivens**, University of Warwick.
- 14:45 Linear quadrupoles with added hexapole fields, **Don Douglas**, N. Kononkov, XianZhen Zhao, W. Xiao, O. Granot, Chemistry, University of British Columbia.
- 15:05 New strategies for IRMPD in a quadrupole ion trap, G. A. Newsome, P.R. Remes, **Gary L. Glish**, University of North Carolina.

15:25 Structures of Proton and Metal Ion-Bound Amino Acids and DNA bases by IRMPD Spectroscopy in the 700 to 2000 cm<sup>-1</sup> Region, *Negar Rajabi*, T. D. Fridgen, Department of Chemistry, Memorial University.

15:45 Unimolecular dissociations of methyl-substituted hydrazine ions, *Anne-Marie Boulanger*<sup>1</sup>, E.E. Rennie<sup>1</sup>, D.M.P. Holland<sup>2</sup>, D.A. Shaw<sup>2</sup>, P.M. Mayer<sup>1</sup>,  
<sup>1</sup>Chemistry, University of Ottawa, <sup>2</sup>Daresbury Laboratory, Daresbury, UK.

**16:05 Discussion**

**16:10 Break**

16:40 Ionizing polymers with protonated amino acids: new fragmentation pathways and thermochemistry, A. Alhazmi, *Paul M. Mayer*, Chemistry, University of Ottawa.

17:00 Creating time and space for better MS//MS analysis: a new scheme for 2D-LC/ESI MS with peptide retention prediction in both dimensions, *Oleg V. Krokhin*, V. Spicer, R. Swivedi, M. Antonovici, M. Harder, K. G. Standing, J. A. Wilkins,  
<sup>1</sup>Manitoba Centre for Proteomics and Systems Biology.

17:20 Hydroxyl radical labeling and ESI-MS/MS for the structural characterization of proteins in solution, *Lars Konermann*, Xin Tong, B. Stocks, The University of Western Ontario.

17:40 Investigations into peptide fragment ions structures using combined ion mobility-mass spectrometry (IM-MS) and tandem mass spectrometry (IM-MS/MS), *Isabel Riba-Garcia*<sup>1</sup>, K. Giles<sup>2</sup>, R.H. Bateman<sup>2</sup>, S.J. Gaskell<sup>1</sup>,  
<sup>1</sup>The University of Manchester, <sup>2</sup>Waters Corporation.

**18:00 Discussion**

**18:30 Dinner**

### Evening Session

*Chair: Orval Mamer*

20:00 High sensitivity absolute quantification of proteins using QconCAT standards and selective peptide derivatisation, *Simon Gaskell*, University of Manchester.

20:20 Identification of protein biomarkers of ovarian cancer using iTRAQ and mass spectrometry: giving voice to “The silent killer”, *Daryl Smith*, K.W. Michael Siu, York University.

20:40 Novel MS-cleavable crosslinkers for structural proteomics, *Christoph H. Borchers*, E.V. Petrotchenko, Protein Centre, University of Victoria.

**21:00 Discussion**

**21:05 Poster Session – please man posters until 23:00**

FT-MS Determination of Deamidation, Li Zhou, *Carol Parker*, Maria E. Warren, Linhong Jing, Cameron O. Scarlett, Xian Chen, UNC-Duke Proteomics Center, University of North Carolina, Chapel Hill, NC.

Novel Off-line Multidimensional LC Method for Separation and Tandem MS Detection of Tryptic Peptides (Abstract), R. van Ling, K. Cook, A. Adam, B. Dolman, *JF Carriere*, E-J Sneekes, R. Swart, Dionex Corp, Dionex Ltd., Dionex Canada Ltd.

A collection of novel isotopically-coded crosslinkers for structural proteomics, **Evgeniy.V. Petrotchenko**, C.H. Borchers, Protein Centre, University of Victoria.

Iodo-Acid disinfection by-products in drinking water: does LC/ESI-MS/MS offer an advantage over GC/NCI-MS?, **Susan Richardson**<sup>1</sup>, F. Fasano<sup>1</sup>, J.J. Ellington<sup>1</sup>, F.G. Crumley<sup>1</sup>, K. Buettner<sup>1</sup>, J.J. Evans<sup>1</sup>, B.C. Blount<sup>2</sup>, L.K. Silva<sup>2</sup>, F.L. Cardinali<sup>2</sup>, M.J. Plewa<sup>3</sup>, E.D. Wagner<sup>3</sup>, G.W. Luther III<sup>4</sup>, T.J. Waite<sup>4</sup>, <sup>1</sup>US EPA, <sup>2</sup>Centers for Disease Control and Prevention, Atlanta, <sup>3</sup>University of Illinois, <sup>4</sup>University of Delaware.

Identification of Fatty Acids Utilizing exact mass and MALDI MSMS on a 4800 tof tof, **Doug Olson**<sup>1</sup>, M. Dauk, M. Smith, A. Ross, NRC Saskatoon.

Analysis of Mycotoxins in Food Matrices using ESI-FAIMS-MS(MS), **Margaret McCooye**<sup>1</sup>, B. Kolakowski<sup>1</sup>, J. Boison<sup>2</sup>, Z. Mester<sup>1</sup>, <sup>1</sup>NRC Institute for National Measurement Standards, <sup>2</sup>Canadian Food Inspection Agency.

Investigating the performance and stability of rapid polarity switching during the quantitative UPLC-ESI-MS/MS analysis of complex mixtures, **George A. Keenan**, Scottish Agricultural Science Agency, Edinburgh.

Comparison of LC-MS-MS methods for quantification of trace levels of fluoroquinolone antibiotics in honey, **David A. Durden**, G. Fernandez, Canadian Food Inspection Agency.

Desorption electrospray tandem mass spectrometry (DESI-MS/MS) on chemical warfare agents, **Paul A. D'Agostino**, **Claude L. Chenier**, C.R. Jackson Lepage, J.R. Hancock, DRDC Suffield.

Quantitative determination of nifedipine in human plasma by high performance liquid chromatography – tandem mass spectrometry using EP10+/HSID interface, **Navgeet Bajaj**, I. Balkhi, N. Hughes, Biovail Contract Research.

Ambient air measurements of BTX and trimethylbenzenes in urban and industrial areas in Ontario using mobile TAGA mass spectrometry, N. S. Karellas, A. C. Ng, **QingFeng Chen**, Ontario Ministry of the Environment.

Human Serum Proteins Fractionated by Preparative Chromatography Prior to LC-MS/MS with an Ion Trap and Controlled Correlation with X!TANDEM, Monika Tucholska, Peter Bowden, Peihong Zhu, **John Marshall**, Department of Chemistry and Biology, Faculty of Engineering, Architecture and Science, Ryerson University. Toronto, Canada.

Bioinformatical Data Mining in Shotgun Proteomics, **John Chakel**, Morten Bern, Christian Ingrell, Alexandre Podtelejnikov, and Ole Vorm, Proxeon, San Mateo, CA and OdenseDenmark.

Preliminary localization of the laulimalide binding site on assembled tubulin, **Melissa Bennett**, G. Slys, D.Schriemer, University of Calgary.

Hydrogen deuterium exchange mass spectrometry to study the transitional state of Ebola virus matrix protein VP40, **Leslie Silva**, M. Vanzile, M.J. Aman, D.C. Schriemer, University of Calgary

System optimization for rapid HDX-MS analysis, **Andrew Percy**, E. Kelly and D. Schriemer, University of Calgary.

Immuno tandem mass spectrometry (iMASS2) assay for clinical proteomics: development and application of iMAS2 for EGFR diagnosis, **Jennifer Reid**<sup>2</sup>, Jian Jiang<sup>1</sup>, C.E. Parker<sup>1</sup>, K.A. Hoadley<sup>1</sup>, C.M. Perou<sup>1</sup>, C.H. Borchers<sup>2</sup>, <sup>1</sup>University of North Carolina, <sup>2</sup>University of Victoria, Genome BC Proteomics Centre.

Targeted imaging by MRM-MALDI, **Derek Smith**, Jun Han, C.H. Borchers, University of Victoria, Genome BC Proteomics Centre.

Proteomics of Membrane Rafts, **Morgan F. Hughes**, Julie P. Deans, David C. Schriemer, University of Calgary.

Purity verification of fluorochemicals using LC-MS-MS, **Jonathan Naile**, University of Saskatchewan.

The use of a parallel CID-Ion Mobility-CID fragmentation technique for structure elucidation in metabolite identification studies, **Jose M. Castro-Perez**, J. Shockcor and K. Yu, Waters Corporation.

Approaches for the confirmation of putative biomarkers using multiple-reaction monitoring(Abstract), **Linda Côté**<sup>1</sup>, Ning Tang<sup>2</sup>, C. Miller<sup>2</sup>, Hongfeng Yin<sup>2</sup>, R. Gudihal<sup>2</sup>, K. Waddell<sup>2</sup>, <sup>1</sup>Agilent Technologies, Montreal, <sup>2</sup>Santa Clara, CA.

## Friday, Nov. 30, Morning Session

*Chair: Simon Gaskell*

- 8:15 Electron detachment dissociation for the analysis of glycosaminoglycan carbohydrates, **Jon Amster**, J. Wolff, F. Leach, University of Georgia.
- 9:00 Duplex and sixplex tandem mass tags for isobaric protein/peptide labelings, **Peter Verhaert**, I.M.O. Finoulst and M.W. Pinkse, Delft University.
- 9:20 Optimizing phosphopeptide analysis to discover host signaling events induced by Salmonella, **Lindsay D. Rogers**, E.C. Boyle, L.J. Foster, Biochemistry, University of British Columbia.
- 9:40 Use of live-cell affinity receptor chromatography (LARC) to capture the activated Fc receptor complex from the surface of live cells, A. Jankowski, **John G. Marshall**, Ryerson University, Toronto.

**10:00 Discussion**

**10:10 Break**

- 10:30 Entropy effects in the dissociation of protein-ligand complexes in the gas phase, **John Klassen**, E. Kotova, University of Alberta.
- 10:50 LC/MS for comprehensive proteome analysis: an update, **Liang Li**, University of Alberta.
- 11:10 Tandem MS by MRM and iMALDI for absolute quantitative and clinical proteomics, **Michael Kuzyk**, A. Jackson, T. Cross, D. Hardie, Juncong Han, B. Shaw, J. Reid, C.H. Borchers, Protein Centre, University of Victoria.
- 11:30 Evaluating reproducibility and similarity in MALDI spectra – applications to several types of problem, M.T. Olson, J.A. Epstein, **Al Yergey**, .
- 11:50 Applications of a high-pressure segmented quadrupole as an ion-mobility spectrometer within a triple-quadrupole mass spectrometer, Y. Guo<sup>1</sup>, B.A. Thomson<sup>1,2</sup>, **K.W. Michael. Siu**<sup>1</sup>, <sup>1</sup>York University, Toronto, <sup>1</sup>MDS Analytical Technologies.

**12:00 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. 1, Morning Session

*Chair: Gordon McKay*

- 8:20 **Lossing Award Presentation:** Where can we go from here? An assessment of the limits of sensitivity, reproducibility and speed of ESI, APCI and MALDI, **Tom Covey**, Brad Schneider, Peter Kovaric, MDS/Sciex.
- 9:05 Identification of xenobiotic metabolites in complex biological matrices using advanced high resolution UPLC/qTof acquisition techniques and multivariate statistical methods, **John P. Shockcor**, J. Castro-Perez, K. Yu, Waters Corp.
- 9:25 High energy collision dissociation and multiple mass defect filters as techniques for more efficient metabolite identification, **Brenda S. Kesler**, Yingying Huang, Thermo Fisher Scientific.
- 9:45 Accurate mass and structure assignment in metabolite identification studies, **Kevin Bateman**, Merck.

**10:05 Discussion**

**10:10 Break**

- 10:40 Real-time signal processing for enhancement of resolution and dynamic range on TOF and QTOF mass spectrometers, **Patrick Perkins**, P. Poupart, Agilent.
- 11:00 Drugs of abuse screening and confirmation of positives for amphetamines by LC/MS/MS: LC/MS/MS compares favourably to both immunoassays and GC/MS, **Jeff Eichhorst**, Saskatchewan Provincial Laboratory.
- 11:20 Fragmentation patterns of fatty acid barium cluster ions and its application to lipidomics, **Nicole Zehethofer**<sup>1</sup>, D. M. Pinto<sup>2</sup>, D.A. Volmer<sup>3</sup>, <sup>1</sup>Dalhousie University, NRC Halifax, <sup>2</sup>Institute for Marine biosciences, <sup>3</sup>NRC HNR.
- 11:40 Exploring UV laser induced dissociation for structural characterization of small molecules, **J.C.Yves LeBlanc**, A. V. Loboda, MDS/Sciex.

**12:30 Adjourn and Lunch**