

LAKE LOUISE XXII

22ST Workshop on Tandem Mass Spectrometry

Thursday, December 3, 2009, Morning Session

Chair: Gary Glish

- 8:20 Introductory Remarks: **Gordon McKay**
- 8:25 Structures and binding energies of noncovalently bound complexes of protonated peptidomimetic nitrogen bases with 18-crown-6, **Mary Rodgers & Yu Chen**, Wayne State University, Detroit.
- 9:10 Using electrons for ion activation in a linear ion trap, **Gary L. Glish**, Takashi Baba, Natalie J. Thompson, & Atim A. Enyenihi, University of North Carolina.
- 9:30 Profiling ion cloud distribution in a quadrupole ion trap mass spectrometer with infrared multiphoton photodissociation, **G. Asher Newsome (Winner of a Lake Louise Workshop Committee Student Travel Award)**, Alfred Z. Zhong & Gary L. Glish, University of North Carolina.
- 9:50 Mass analysis in islands of stability: a cure for bad quadrupoles?, **Don Douglas**, Department of Chemistry, The University of British Columbia.

10:10 Discussion

10:20 Break

- 10:35 **Lossing Award Presentation (Supported by Varian):** Water cluster ions in collision: Newton's Cradle, **Orval Mamer¹**, Alain Lesimple¹ & Matthew Price-Gallagher², ¹McGill University MS Facility, ²HydroElectron Ventures.
- 11:10 Using tandem mass spectrometry to establish an absolute electrochemical scale, **William A. Donald (Winner of the Research Scientific Services supported Lake Louise Student Travel Award)** & Evan R. Williams, Dept. of Chem, University of California, Berkeley.
- 11:30 The potential of the high sensitivity porous sprayer in small molecule analysis (CE-HSPS-MS), **John C. Hudson¹**, Beckman Coulter Inc., Brea, CA.
- 11:50 Pushing the limits of protein coverage in HPLC/MS/MS for influenza hemagglutinin, Daryl G. S. Smith, Marybeth Cameron & **Terry D. Cyr**, Health Canada.

12:10 Discussion

12:30 Lunch (in the Fairview Room)

Afternoon Session

Chair: Simon Gaskell

- 14:00 Top down proteomics: has its time now come?, **Neil Kelleher**, & the Top Down Development Team, Dept. of Chem., University of Illinois.
- 14:45 Progress in top-down and bottom-up mass spectrometry for structural studies of proteins in solution, **Lars Konermann¹**, Jingxi Pan¹, Yan Pan¹, Bradley B. Stocks¹, Christoph H. Borchers² & Jun Han², ¹Depts of Chem & Biochem, The University of Western Ontario, London, ON, ²University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

15:05 Making progress – crosslinking combined with MS for structural proteomics, Jenya Petrotchenko, Jason Serpa & **Christoph Borchers**, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

15:25 Discussion

15:35 Break

Chair: Lars Konermann

15:50 Determining protein quaternary structures using constraints from gas-phase measurements, **Brandon T. Ruotolo**, Dept. of Chem, University of Michigan,.

16:35 Tandem MS and ion-mobility coupled tandem MS experiments for in vivo metabolite identification, **Andrew Baker**, Mass Spectrometry Applications, Waters Corporation, Pleasanton, CA.

16:55 Enhanced proteomic analyses using high field asymmetric waveform ion mobility on an LTQ-Orbitrap mass spectrometer, **Éric Bonneil**, Tara Muraore-Schreiber, Gaele Bridon & Pierre Thibault, Institute for Research in Immunology & Cancer, Université de Montréal.

17:15 Detailed kinetic studies of solution-phase protein unfolding using time-resolved ESI and IMS/MS with a DMA/QTOF mass spectrometer, **John van Nostrand**¹, Tamanna Rob¹, Bruce Thomson^{1,2}, Derek Wilson¹, K. W. Michael Siu¹, ¹Centre for Research in Mass Spectrometry Toronto, ON, ²MDS Analytical Technologies, Concord, ON.

17:35 Discussion

18:00 Dinner

Evening Session

Chair: Orval Mamer

20:00 The rationale for the the contents of Practical Aspects of Trapped Ion Mass Spectrometry, Volumes 4 and 5, **Ray March**¹ & John Todd², ¹Trent University, Peterborough, ON, ²The University of Kent, Canterbury, Kent, England.

20:45 Discussion

20:50 Poster Session – please man posters until 23:00

Direct analysis of volatile methylsiloxanes in gaseous matrixes using atmospheric pressure chemical ionization-tandem mass spectrometry, K. Badjagbo, A. Furtos, **Mehran Alaei**, S. Moore & S. Sauvé, Water Science & Technology Directorate, Environment Canada, Burlington, ON.

Maximizing performance of conventional time of flight technology: resolution, accuracy and speed, **Richard Barry**, Michael Ugarov and all, Agilent.

Tandem mass spectrometric dissociation behaviour of 30 novel Gemini surfactants and preliminary LC-MS/MS method development, **Joshua Buse**¹, Ildiko Badea¹, Ronald E. Verrall² & Anas El-Aneid¹, ¹College of Pharmacy and Nutrition, University of Saskatchewan, SK, ²Dept. of Chem., University of Saskatchewan, Saskatoon, SK.

Microfluidics based integration of sample prep and liquid chromatography for rapid MS/MS based characterization of N-linked glycans from therapeutic antibodies, **Maggie A. Bynam**, Javier Satulovsky, Hongfeng Yin & Kevin Killeen, Agilent.

Combined tandem MS/ion mobility studies of peptide ions, **Ross Chawner** & Simon Gaskell, University of Manchester.

MRM based, multiplexed, absolute, quantitation of 63 proteins in human plasma, Michael A. Kuzyk, Juncong Yang, **Tyra J. Cross**, Derek Smith, Angela Jackson, Darryl Hardie, N. Leigh Anderson & Christoph Borchers, Genome BC Proteomics Centre, University of Victoria, Victoria, BC.

Chemical warfare agent analysis by ion mobility spectrometry and tandem mass spectrometry, **Paul A. D'Agostino** & Claude L. Chenier, DRDC Suffield, AB.

A new approach to the analysis of nicarbazin and ionophores in eggs by LC-MS/MS, Jasna Dmitrovic & **David Durden**, Canadian Food Inspection agency, Calgary, AB.

Is acetonitrile reduced to ethylamine during ESI? Effect of ethylamine on analysis of veterinary antibiotics, **David Durden** & Jasna Dmitrovic, Canadian Food Inspection agency, Calgary, AB.

The elucidation of histone methyltransferase target amino acid residues and downstream modification events by quantitative mass spectrometry, **Shannon Eliuk**, Feixia Chu, Barbara Panning & Al Burlingame, Dept. of Pharmaceutical Chemistry, University of California at San Francisco.

Development of an HPLC-MS-MS method for the determination of thymine photoproducts, **Brian Fahlman**¹, Ed Krol¹, Kerry Peru², & John Headly², ¹College of Pharmacy and Nutrition, University of Saskatchewan, SK, ²Environment Canada.

Protonated tryptophan ions and neutrals in the gas phase, **Joshua A. Gregersen**, & Frantisek Turecek, Dept. of Chem., University of Washington.

Application of UV photodissociation on a QqTOF: generation and detection of unique fragment ions on an LC-timescale, (presented by **Larry Campbell** & **Bruce Thomson**), Changtong Hao¹, J. C. Yves Le Blanc², **Bruce A. Thomson**^{1,2}, K. W. Michael Siu¹ & Alexander V. Loboda², ¹York University, Toronto, ON, ²MDS SCIEX, Concord, ON.

Plant hormone profiling – powerful tool for plant genomic research, , Suzanne R. Abrams, **Xiumei Han**, Steve Ambrose, Stacey Owen, Vera Cekic, Monika Lafond, Ken Nelson, Pearla Gai & L. Irina Zaharia, Plant Biotechnology Institute, NRC, Saskatoon, SK.

Combining unbiased metabolic profiling with targeted analysis of specific metabolites using high resolution mass spectrometry, a step forward in metabolomics, Albert Koulman¹, Martin Hornshaw², Gary Woffendin², Vinod K. Narayana¹, Helen Welchman², Julain Phillips³, Catharina Crone⁴ & Dietrich A. Volmer¹, presented by **Stephen Hassan**⁵, ¹MRC Human Nutrition Research, Cambridge, UK & Thermo Fisher Scientific, ²Hemel Hempstead, UK, ³San Jose, USA, ⁴Bremen, Germany, & ⁵Mississauga, ON.

Development of a novel mass-spectrometry identifiable cross-linker and application to a 34K – actin protein system, **Lisabeth L. Hoffman**¹, Paul Griffin¹, Marcus Fechheimer¹, Evgeniy Petrotchenko², Christoph H. Borchers² & I. Jon Amster¹, ¹University of Georgia, Athens, Georgia, ²Genome BC Proteomics Centre, University of Victoria, Victoria, BC.

Demonstrating a novel triple play with CID/ETD decision tree strategy for proteomics experiments on a new dual-cell linear ion trap, **Julie A. Horner**, Roger G. Biringer & Andreas FR Hühmer, Thermo Fisher Scientific, San Jose, Ca.

Determination of cis- and trans-resveratrol and polydatin in dietary supplements using the Varian 500-MS LC/MS ion trap mass spectrometer, Tiffany Payne¹ & **James Neal-Kababick**², ¹Varian Inc, Walnut Creek, CA, ²Flora Research Laboratories, Grants Pass OR.

METLIN personal compound database and Library: enhanced to include MS/MS spectral libraries for more confident identification, **Julie Marr**, Steve Fischer and all, Agilent.

Quantization of the alpha- and beta-Asp7 isoforms of Alzheimer's amyloid-beta-(1-16) peptide by MS/MS, Maria I. Indeykina¹, Igor A. Popov^{1,2}, Sergey A. Kozin³, Alexey S. Kononihin^{1,2} & **Evgeny N. Nikolaev**^{1,2,3}, ¹Institute for Energy Problems of Chemical Physics Russian Academy of Science, ²Institute for Biochemical Physics Russian Academy of Science, ³Institute for Biomedical Chemistry Russian Academy of Medical Science.

H/D exchange mass spectrometry with top-down electron capture dissociation for characterizing structural transitions of proteins in solution, **Jingxi Pan**¹, Jun Han², Christoph H. Borchers² & Lars Konermann¹, ¹Dept. of Chem., The University of Western Ontario, London, ON, ²Genome BC Proteomics Centre, University of Victoria, Victoria, BC.

MALDI TOF/TOF MS3 analysis of isotopically-coded CID-leavable crosslinkers, **Evgeniy Petrotchenko** & Christoph Borchers, Genome BC Proteomics Centre, University of Victoria, Victoria, BC.

What's in the pool? A comprehensive identification of disinfection by-products and assessment of mutagenicity of chlorinated and brominated swimming pool water, **Susan Richardson**¹, David M. DeMarini², Manolis Kogevinas^{3,4,5,6}, Pilar Fernandez⁷, Esther Marco⁷, Carolina Lourencetti⁷, Cara Balleste⁷, Dick Heederik⁸,

Kees Meliefste⁸, A. Bruce McKague⁹, Ricard Marcos¹⁰, Laia Font-Ribera^{3,4}, Joan O. Grimalt⁷, & Cristina M. Villanueva^{3,4,5}, ¹U.S. EPA, National Exposure Research Laboratory, Athens, GA, ²U.S. EPA, National Health and Environmental Effects Research Laboratory, RTP, NC, ³Centre for Research in Environmental Epidemiology, Barcelona, Spain, ⁴Municipal Institute of Medical Research, Barcelona, Spain, ⁵CIBER Epidemiología y Salud Pública, Barcelona, Spain, ⁶National School of Public Health, Athens, Greece, ⁷Institute of Environmental Assessment and Water Research, Barcelona, Spain, ⁸Institute for Risk Assessment Sciences, Utrecht University, ⁹CanSyn Chem. Corp., Toronto, Canada, ¹⁰Universitat Autònoma de Barcelona, Bellaterra, Cerdanyola del Vallès, Spain.

Influence of thioketo and methyl substitution on the structures and properties of uracil, David Nei¹, Tolulope E. Akinyemi¹, **Mary T. Rodgers**¹, Jos Oomens² & Jeff Steill², ¹Wayne State University, Detroit, ²FOM Institute for plasma physics “Rijnhuizen”, Nieuwegein, The Netherlands.

An isotopically-coded CID-cleavable biotinylated crosslinker: CBDPS for structural proteomics, **Jason J. Serpa**, Evgeniy V. Petrotchenko & Christoph H. Borchers, Proteomics Centre, Victoria, BC.

High sensitivity and mass resolution on a QqTOF mass spectrometer, Alexandre Loboda, Igor Chernushevich, Nic Bloomfield & **Bruce Thomson**, MDS Analytical Technologies.

Development and validation of a LC-MS/MS assay for prostaglandin F_{2α} (PGF_{2α}) in bovine milk. **Raymond Zielinski** & Pamela L. Boner, Pfizer Animal Health Veterinary Medicine Research & Development, Kalamazoo, Michigan.

Friday, Dec. 4, Morning Session

Chair: Michael Siu

- 8:20 Potential glioblastoma multiforme biomarkers: from discovery, verification to functional characterization, Leroi V. DeSouza¹, Joydeep Mukherjee², G. Declan Williams¹, Leroi V. DeSouza¹, Abhijit Guha², **K. W. Michael Siu**¹, ¹York University, Toronto, ON, ²Hospital for Sick Children, Toronto ON.
- 8:40 Profiling global changes in the phosphoproteome of epithelial cells following the inhibition of Erk1/2 map kinase pathway, **Mathieu Courcelles (Winner of the Waters Canada supported CSMS Student Travel Award)**, L. Julien C. Voisin, S. Lemieux, S. Meloche & P. Thibault, Université De Montréal, Montréal.
- 9:00 Identification and verification of putative biomarkers for ovarian cancer using a MS-based biomarker discovery pipeline, **Sarah Elschenbroich (Winner of the Thermo Fisher supported CSMS Student Travel Award)**, Vladimir Ignatchenko¹, Patricia A. Shaw², Igor Jurisica^{3,4} & Thomas Kislinger¹, ¹Dept. of Medical Biophysics, Ontario Cancer Institute, University of Toronto, ON, ²Dept. of Laboratory Medicine and Pathology, University of Toronto, ON, ³Division of Signaling Biology, Toronto, ON, ⁴?, University of Toronto, ON
- 9:20 Assay development for the determination of phosphorylation stoichiometry: analysis of breast cancer signalling pathways, **Dominik Domanski (Winner of the MDS/SCIEX supported CSMS Student Travel Award)**, M. Kuzyk & C. Borchers, **Genome BC Proteomics Centre**, University of Victoria, BC.

- 9:40 Discussion**
9:55 Break
- 10:15 The role of tandem MS in proteome-wide absolute quantification of proteins, **Simon Gaskell**¹, Rob Beynon², Simon Hubbard³, Chris Grant³, Paul Sims³, ¹Queen Mary, University of London, ²University of Liverpool, ³University of Manchester.
- 10:35 Ultra-high-performance nano LC-MS/MS analysis of complex proteomic samples, **Evert-Jan Sneekes**, Dionex Canada Ltd.
- 10:55 A MALDI FT-ICR-MS/MS study of metal ion attachment to peptides, **Karl J. Jobst**¹ (Winner of a Lake Louise Workshop Committee Student Travel Award) Johan K. Terlouw¹, Theo M. Luiders² & Peter C. Burgers², ¹Dept. of Chem., McMaster University Hamilton, ON, ²Laboratory for Neuro-Oncology, Erasmus Medical Center, Rotterdam, The Netherlands.
- 11:15 A priori recognition of post-translationally modified peptides, **Al Yergey**, Jonathan Epstein, Matthew Olson, Paul Blank, Peter Backlund & Aaqron Catlett, NIH.
- 11:35 New sample handling methods for shotgun proteome analysis by LC/MS, **Nan Wang** & Liang Li, University of Alberta, AB.
- 11:55 Optimization of chromatographic separation space for exhaustive LC-MS/MS analysis in bottom-up proteomics, **Oleg Krokhin**, Dept. of Internal Medicine, University of Manitoba..
- 12:15 Discussion**
12:30 Lunch
13:30 Geology of Lake Louise, with Bob Davidson, in lobby
14:00 Information walk, with Bob Davidson, up lake
16:30 Broomball: Canada vs. The World
18:30 Banquet – Mount Temple Ballroom A

Sat., Dec. 5, Morning Session

Chair: Gordon McKay

- 8:30 Quantification of abscisic acid and abscisic acid metabolites in various plant tissues by ultra performance liquid chromatography tandem mass spectrometry, **Xiumei Han**, Vera Cekic, Monika Lafond, Stacey Owen, Steve Ambrose, L. Irina Zaharia & Suzanne R. Abrams, Plant Biotechnology Institute, NRC, Saskatoon, S.K.
- 8:50 Using targeted charge separation for quantifying biotherapeutics as whole molecules, **J. Larry Campbell**¹, J. C. Yves Le Blanc¹, Changtong Hao² & K. W. Michael Siu², ¹AB Sciex, Concord, ON, ²Center for Research in Mass Spectrometry, York University, Toronto, ON.
- 9:10 Electrospray coupled microfluidics for the 'masses', Tamanna Rob, Peter Liuni, Yanfang Liang & **Derek J. Wilson**, Chem. Dept., York University, Toronto, ON.
- 9:30 Microfluidics integration of sample preparation and liquid chromatography for Rapid MS/MS based characterization of N-linked glycans from therapeutic antibodies, **Maggie A. Bynum**, Javier Satulovsky, Hongfeng Yin & Kevin Killeen, Agilent Laboratories, Santa Clara, CA.
- 9:50 Discussion**

10:05 Break

- 10:25 Technical innovations and practical applications of a novel dual-cell linear ion trap, **Julie A. Horner**, Jae C. Schwartz & August A. Specht, Thermo Fisher Scientific, San Jose, CA.
- 10:45 Phytoforensic detection and characterization of novel clandestine PDE-5 inhibitor analogue drugs in dietary supplements utilizing automated turboDDS MSn, **James Neal-Kababick**, Flora research laboratories.
- 11:05 Comparison of electron-induced dissociation methods for top-down protein analysis for structural and sequence information, Rinat Abzalimov¹, Desmond A. Kapln², **Mike L. Easterling**², Christopher Thomas², Jeremy Wolff² & Igor A. Kaltashov¹, ¹The University of Massachusetts, Amherst, ²Bruker Daltonics, Inc., Bilerica, MA.
- 11:25 LC/MS/MS identification of new water disinfection byproducts, Feng Qin, Yuli Zhao, Jessica Boyd, Wenjun Zhou & **Xing-fang Li**, Faculty of Medicine and Dentistry, University of Alberta, AB.
- 11:45 Formation of Iodo-DBPs from x-ray contrast media: update on mechanisms and toxicity of reaction products, **Susan Richardson**¹, Stephen E. Duirk¹, Cristal Lindell¹, Christopher Cornelison¹, Thomas A. Ternes², Jennifer Kormos² & Michael J. Plewa³, ¹U. S. EPA, National Exposure Research Laboratory, Athens, GA., ²Federal Institute of Hydrology (BfG), Koblenz, Germany, ³Universtiy of Illinois, Urbana, IL.

12:05 Discussion

12:15 Adjourn and Lunch