

LAKE LOUISE XXV

25th Workshop on Tandem Mass Spectrometry

Thursday, November 29, 2012, Morning Session

8:00 Introductory Remarks: **Gordon McKay**

Chair: Gordon McKay *Peptides and Proteins 1*

8:10 Determination of site-specific protein disulfide bond reduction potentials by top-down FT-ICR MS, **Alan Marshall**, Jenna Scotcher and Nicolas L. Young, National High Magnetic Field Laboratory, Florida State University.

8:50 Synergism between IRMPD spectroscopy and DFT calculations in structural elucidation of peptide fragment ions, Junfang Zhao, Udo H. Verkerk, Justin Kai-Chi Lau, Alan C. Hopkinson and **K. W. Michael Siu**, Department of Chemistry and Centre for Research in Mass Spectrometry, York University, Toronto, ON, Canada.

9:10 Remarkable age-related protein post-translational modifications identified by FT-MS, **Ann English**, Concordia University.

9:30 Conflict among the peaks: destructive interference can erode accuracy of HDX measurements in FT-MS, Kyle Burns¹, Martial Rey¹, **David Schriemer**¹ and C. J. Baker², ¹University of Calgary, ²Cultivated Code Inc.

9:50 Discussion
Coffee Break

Chair: Peter Verhaert *Peptides and Proteins 2*

10:20 Tandem mass spectrometry, the enabling tool for protein footprinting, **Michael Gross**, Washington University.

11:00 The role of tandem MS in a comprehensive metabolome profiling workflow, **Liang Li**, University of Alberta.

11:20 25 years of tandem MS in structural proteomics, **Christoph Borchers**, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

11:40 Conformer selection and intensified dynamics during catalytic turnover in chymotrypsin, **Peter Liuni**¹ (Winner of the **Waters** supported **CSMS Student Travel Award**), Araby Jeganathan¹ and Derek J. Wilson^{1,2}, ¹York University Department of Chemistry, Toronto, Canada, ²Center for Research in Mass Spectrometry, Toronto, Canada.

12:00 Discussion

12:30 Lunch (in the Fairview Room)

Afternoon Session

Chair: Lars Konermann *Sponsor Talks*

14:00 A quarter of a century of MS/MS – sectors, tandem quads and hybrids, **Mike Morris**, Waters.

14:20 25 years of mass spec innovation driven by market needs, **Darlene Solomon**, Agilent Technologies Inc.

14:40 The evolution of MS/MS over the last 25 years from quadrupoles and ion traps to orbitraps, **Ian Jardine**, Thermo Fischer Scientific.

15:00 Fun ways to probe ion structure and mobility behaviour using differential mobility spectrometry with MS/MS, **Larry Campbell**, AB Sciex.

15:20 Discussion

Coffee Break

Chair: Paul Mayer **Biological/Environmental Applications**

- 15:50 Electron capture dissociation to disulfide, sulfur-selenium, and diselenide bound peptides, **Huilin Li** (Winner of a **Lake Louise Workshop ‘All Sponsor Supported’ Student Travel Award**) and Peter B. O’Connor, University of Warwick.
- 16:10 Identifying targeted cysteine residues during redox signalling in *Fusarium graminearum*, **Christof Rampitsch**, Agriculture and AgriFood Canada.
- 16:30 Full scan tandem MS methods for the identification of novel pollutants, **Paul Chiarelli**, Loyola University.
- 16:50 Tandem MS in discovery of new toxicologically important disinfection byproducts in drinking water, **Xing-Fang Li**, University of Alberta.
- 17:10 New strategies for high spatial resolution imaging mass spectrometry of phospholipids and other key metabolites, Aurélien, Heath Patterson, Martin Dufresne and **Pierre Chaurand**, Dept. of Chemistry, University of Montreal.
- 17:30 Discussion
- 18:00 Dinner: Mt. Temple C

Evening Session

Chair: Michael Siu **Tandem MS: History and Importance for Society**

- 20:00 The mass appeal of our science: using tandem MS to address fundamental questions, **Simon Gaskell**, Queen Mary University of London.
- 20:30 Ion trap tandem mass spectrometry: history and contributions to science, **Raymond E. March**, Trent University, Peterborough, ON.
- 21:00 **Poster Session – authors are required to be present until 23:00**
- Metabolic profiling of chicken muscles to evaluate the effect of chilled conditioning, **Michel Aliani**, University of Manitoba.
- Molecular weight determination of poly(ethylene glycol) in biological samples by reverse phase LC/MS with in-source fragmentation, **Mark Bolgar**, Brian Redding, Guodong Chen and Bethanne Warrack, Bristol-Myers Squibb, ew Brunswick, NJ.
- Computer aided interpretation of lipid structures from TOF/TOF mass spectra, **Robert B. Cody**, JEOL USA, Inc., Peabody, MA, USA.
- A quantitative and selective analysis of Aldosterone and Cortisol in plasma by LC-MS/MS for clinical research, **Linda Côté**, Agilent Technologies Inc.
- The development of lipid derivitization techniques that operate in-line with MS and MS/MS, **Jonathan Curtis**¹, Samuel M. Mugo², Chenxing Sun¹, Sabiqah Tuan Anuar¹, Yuan-Yuan Zhao¹
¹Department of Agriculture, Food and Nutritional Sciences, University of Alberta, ²Grant MacEwan University, Edmonton AB.
- Database of ion mobility & tandem mass spectrometric data: characterization of chemical warfare agents, hydrolysis products & related compounds, **Paul A. D’Agostino**, DRDC Suffield, Canada.
- Proposed mechanism for the formation of a unique positively charged [M-H]⁺ during MALDI-MS analysis of novel antineoplastic curcumin analogues and discrepancies in the MS/MS fragmentation behaviour between [M-H]⁺ and [M+H]⁺, **Hanan (Elsayed) Awad**¹, L. Usher¹, M. J. Stoudemayer², Joe. H. Banoub³, A. Cohen⁴, U. Das¹, J. Amster², J. Dimmock¹, and A. El-

Aneed¹, ¹College of Pharmacy and Nutrition, University of Saskatchewan, ²Department of Chemistry, University of Georgia, Athens, GA, USA, ³Fisheries and Oceans Canada, Science Branch, N.A.F.C., Canada, ⁴Proteomics Core Facility, Clinical Research Centre, Dalhousie University, Halifax, NS, USA.

Diamond nanoparticles as novel matrices for matrix-assisted laser desorption/ionization (MALDI) analysis, **Erica Friesen**¹, Haixia Zhang², Joshua Buse¹, Jackson Chitanda¹, Randy Purves² and Anas El-Aneed¹, ¹College of Pharmacy and Nutrition, University of Saskatchewan, ²Mass Spectrometry Laboratory, National Research Council of Canada, Saskatoon SK, Canada.

ESI/MS/MS analysis of neonicotinoid insecticides in Canadian prairie agricultural wetlands, **John Headley**¹, Christy Morrissey¹, **Kerry Peru**¹, Jonathan Bailey¹, Matthew Hauck² and Allan Cessna³, ¹Environment Canada, Water Science and Technology Directorate, Saskatoon, SK, Canada, ²University of Saskatchewan, Saskatoon, SK, ³Agriculture and AgriFood Canada, Saskatoon, SK.

A comprehensive automated screening method for synthetic cannabinoids in serum using an LC-MS ion trap, L. M. Huppertz, S. Vogt, S. Kneisel and J. Kempf (presented by **Jim Kapron**), Bruker.

What MS/MS experiments tell us about the mechanism of electrospray ionization, **Lars Konermann**, The University of Western Ontario.

Quantification of core signalling pathway proteins in glioblastoma multiforme cell lines by multiple reaction monitoring standardized with QconCAT, **Stefanie Maedler**¹, Declan Williams¹, Ajay Matta², Leroi V. DeSouza¹ and K. W. Michael Siu¹, ¹York University, ²Samuel Lunenfeld Research Institute, Toronto ON.

Generation and reactions of atomic metal anions, **Paul Mayer**, A. Mungham, D. Hassan, J. Roy, J. Butson and J. Halavachizedah, University of Ottawa.

Novel photo-reactive crosslinking reagents for structural proteomics, **Evgeniy Petrotchenko**, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Differential surface modification for the characterization of prion protein aggregates, **Jason J. Serpa**, Genome BC Proteomics Centre, University of Victoria.

Time-of-flight mass spectrometry: from niche to mainstream, **K. G. Standing**, Dept. of Physics & Astronomy, University of Manitoba.

Collision-induced dissociation of carboxylic acid anions, **Robert L. White**, J. Stuart Grossert and Elizabeth A. L. Gillis, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia.

Determination of total metabolite concentration as a means of metabolome sample normalization and sample loading optimization in mass spectrometry-based metabolomics, **Yiman Wu** & Liang Li, University of Alberta.

Friday, Nov. 30, Morning Session

Chair: Albert Heck **Biopharmaceuticals**

8:00 Overview of mass spectrometry for the characterization of biopharmaceutical antibodies, **Paul Schnier**, Amgen, CA.

8:40 Top-down approaches characterizing biopharmaceutical antibodies, **Yury Tsybin**, EPFL Lausanne.

- 9:00 De novo protein sequencing of monoclonal antibodies, **Wendy Sandoval**, Genentech.
- 9:20 Mass spectral characterization of TCEP-induced cleavage of protein therapeutics, **Bethanne Warrack**, Peiran Liu, Mark Bolgar, Guodong Chen, Wei Ding, Yunping Huang, Li Tao, Wei Wu and Reb Russell, Bristol-Myers Squibb, Princeton, NJ.
- 9:40 Native MS for the characterization of biopharmaceutical antibodies, **Albert Heck**, Netherlands Proteomics Centre, Utrecht University, Utrecht, the Netherlands.
- 10:00 Discussion
Coffee Break

Chair: Paul Mayer **Biomedical**

- 10:30 Structural investigation of bacterial lipopolysaccharides and neoglycoconjugate vaccines by MS and tandem MS, **Joseph Banoub** (Winner of the **Lossing Award** sponsored by **Agilent Technologies Inc.**), Dept. of Fisheries and Oceans, Science Branch, Special Projects, Government of Canada.
- 11:10 Challenges and solutions in large molecule regulated bioanalysis using high resolution MS, **Fabio Garofolo**, Algorithme Pharma.
- 11:30 Profiles not panels: visualizing LC/MS & LC/MS/MS for urinary steroids analysis, **Alfred Yergey**¹, Christopher Crutchfield¹ and Matthew Olson², ¹NICHD, NIH, ²Dept. Pathology, Johns Hopkins Medical School.
- 11:50 Selective derivatization and high resolution MS characterization of plasmalogen glycerophospholipids in primary and metastatic colon adenocarcinoma cell lines, **Cassie Fhaner** (Winner of the **Research Scientific Services** supported **Lake Louise Student Travel Award**), Sichang Liu and Gavin E. Reid, Department of Chemistry, Michigan State University.
- 12:10 Discussion
- 12:30 Lunch
- 13:30 Geology of Lake Louise, with Bob Davidson, in lobby
- 14:00 Informative walk up the lake with Bob Davidson
- 16:30 Broomball: Canada vs. The World – meet in lobby at 4:15 P. M.
- 18:00 Cocktails & entertainment – Victoria Ballroom
- 19:00 Banquet – Victoria Ballroom

Sat., Dec. 1, Morning Session

Chair: Lars Konermann **Instrumentation**

- 8:00 LC-MS/MS may not be the gold standard for quantitative analysis: case study illustrating rapid and cost effective mass spectrometric methods in tissue culture matrix, **Joshua Buse**¹, Haixia Zhang², Steve Ambrose², Randy Purves², Christopher C. Mulligan³, Jon Bailey⁴, Kerry Peru⁴, John Headley⁴, Ronald E. Verrall⁵ and Anas El-Aneed⁵, ¹Drug Design & Discovery Group, College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, Canada, ²Mass Spectrometry Laboratory, NRC of Canada, Saskatoon, SK, Canada, ³Department of Chemistry, Illinois State University, Normal IL, USA, ⁴Aquatic Contaminants Research Division, Water Science and Technology Directorate, Science and Technology Branch, Environment Canada, Saskatoon, SK, ⁵Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada.
- 8:20 Reaching the holy grail of CID – C12 precursor ion selection and 20 keV ELab: from MALDI-Linear TOF/RTOF- to MALDI-Spiral TOF/RTOF-MS, **Guenter Allmaier**, Vienna University of Technology.
- 8:40 Real-time aerosol analysis with tandem mass spectrometry, **Gary Glish**, University of North Carolina, Chapel Hill, NC.

- 9:00 “Going multiple” – multiple electrosprays generated from a single microstructured fibre, **Richard Oleschuk**, Queen’s University.
- 9:20 In-gel microwave-assisted acid hydrolysis of proteins and its combination with LC-ESI MS/MS for mapping protein sequences, **Difei Sun** (Winner of a **Lake Louise Workshop ‘All Sponsor Supported’ Student Travel Award**) & Liang Li, University of Alberta.
- 9:40 Analysis of methamphetamine and its metabolite, amphetamine by chiral CESI-MS, **John C. Hudson**, Beckman Coulter Inc., Canada.
- Discussion
- 10:00 Coffee Break
- Chair: Gary Glish **Peptides and Proteins 3**
- 10:30 Mass spectrometry based profiling of ATPases in the biofuel producing bacterium, *Clostridium stercorarium*, **Peter Mcqueen** (Winner of the **AB Sciex supported CSMS Student Travel Award**), John Schellenberg, Richard Sparling, David Levin, Oleg Krokhin and John Wilkins, University of Manitoba, Winnipeg, Manitoba.
- 10:50 Characterization of residual structure in the intrinsically disordered protein Tau, **Shaolong Zhu** (Winner of the **Thermo Fisher supported CSMS Student Travel Award**), Tamanna Rob and Derek Wilson, York University, Center for Research in Mass Spectrometry, Toronto, Canada.
- 11:10 Quantitative proteomics of post-translational modifications, **Daniel Figeys**, University of Ottawa.
- 11:30 Triple X proteomics: universal tools for peptide affinity capture, **Oliver Poetz**, Natural and Medical Sciences Institute at the University of Tübingen, Germany.
- 11:50 (Tandem) mass spectrometry approaches to discover bioactive peptides from complex natural sources. The amphibian defensive skin secretion as model, Martijn Pinkse, Geisa Caprini Evaristo & **Peter Verhaert**, Analytical Biotechnology/Innovative Peptide Biology Group and Netherlands Proteomics Centre, Dept. of Biotechnology, TUDELFT, Delft, The Netherlands.
- 12:10 Discussion
- 12:30 Lunch