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 Schriemer¹ 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 Liuni¹ (Winner of the Waters supported CSMS Student Travel Award), Araby Jeganathan¹ and Derek J. Wilson¹,² 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, New Brunswick, NJ.

Computer aided interpretation of lipid structures form 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. Amster³, J. Dimmock¹, and A. El-
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 Maedler1, Declan Williams1, Ajay Matta2, Leroi V. DeSouza1 and K. W. Michael Siu1, 1York University, 2Samuel Lunenfeld Research Institute, Toronto ON.


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, Christopher Crutchfield and Matthew Olson, 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, Haixia Zhang, Steve Ambrose, Randy Purves, Christopher C. Mulligan, Jon Bailey, Kerry Peru, John Headley, Ronald E. Verrall and Anas El-Aneed, 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