LAKE LOUISE XXVII

27th Workshop on Tandem Mass Spectrometry

Thursday, December 4, 2014

8:00 Introductory Remarks: Lars Konermann

Glycobiology	Chair	Kristina	Hakansson
Ulveuluev	Chan.	MISUIIa	Hananssun

- 8:10 Mass Spectrometry reveals amazingly cool features of glycans, *Catherine E. Costello*, Boston University, School of Medicine.
- 8:50 Quantitative glycomics and monitoring health, Carlito Lebrilla, University of California, Davis.
- 9:10 Information rich MS/MS strategies for glycopeptide analysis, *Eric D. Dodds*, University of Nebraska, Lincoln.
- 9:30 LC-MS/MS and MS/MS of permethylated glycans, Yehia Mechref, Texas Technical University.
- 9:50 Discussion

 Coffee Break

Lipids, Metabolites, and Biomarkers Chair: Gary Glish

- 10:20 Biomarker discovery to clinical applications: Down to basics, *Christiane Auray-Blais*, Université de Sherbrooke.
- 10:40 Identifying reactive metabolite protein targets using click chemistry, *André LeBlanc* (CSMS Travel Award Winner, sponsored by Sciex), Université du Québec à Montreal.
- 11:00 LC-MS analysis of common mycotoxins in blood for exposure monitoring, *Dajana Vuckovic*, Concordia University, Montreal.
- Analysis of DNA oxidation in cells by LC-ESI-MS/MS, Guru Swamy Madugundu (Winner of a Lake Louise Travel Award, sponsored by Research Scientific Services), University of Sherbrooke.
- Top-down tandem MS analysis of human aqueous humor yields biomarkers, *Bharath Kumar Raghuraman* (Winner of a Lake Louise 'All Sponsor' Travel Award), Delft University of Technology.
- 12:00 Discussion
- 12:10 Workshop group picture
- 12:30 Lunch (in the Fairview Room)

Photo-Dissociation and Ion-Photon Interactions Chair: Albert Heck

- 14:00 Ultraviolet photodissociation for analysis of biomolecules, *Jenny Brodbelt*, University of Texas at Austin.
- Molecular structure of CID and ETD product ions by ion spectroscopy, *Jos Oomens*, Radboud University Nijmegen.
- 15:00 Native chromophore excitation energy transfer for protein structure determination, *Ryan Julian*, University of California, Riverside.
- 15:20 Photodissociation, fluorescence and FRET to probe trapped biomolecules, *Rebecca A. Jockusch*, University of Toronto.
- 15:40 Discussion

 Coffee Break

Electron-Mediated Dissociation Chair: Susan Richardson

- 16:10 Electron capture dissociation mass spectrometry for high throughput glycoproteomics, *J. Larry Campbell*, AB Sciex.
- 16:30 Alternative charge carriers in electron-based MS/MS, *Kristina Hakansson*, University of Michigan, Ann Arbor.
- 16:50 Electron induced dissociation (EID) for lipids and steroids, *Jace Jones*, University of Maryland.
- 17:10 Discussion
- 18:00 Dinner: Mt. Temple

Instrumentation Chair: Peter Verheart

- 19:30 Fringing field mass spectrometry (Lossing Award Lecture), James Hager, AB Sciex.
- Novel data independent analysis methods for pathway characterization, presented by *Michael Blank*, Thermo Fisher Scientific.
- TrEnDi: a tool to enhance sensitivity in proteomics and lipidomics, *Jeff Smith*, Carleton University, Ottawa.
- The effective potential for ion motion in a quadrupole field revisited, *Don Douglas*, University of British Columbia, Vancouver.

21:10 Poster Session—authors are required to be present until 23:00

- Bioanalytical strategies for investigation of denovo steroid synthesis and androgen withdrawal in prostate in vitro and in vivo, *Hans Adomat*¹, Steven Pham¹, Dong-Sheng Ming¹, Mei Yieng Chin¹, Subrata Deb² and Emma S. (Tomlinson) Guns¹, ¹Vancouver Prostate Centre, ²Roosevelt University, Chicago.
- Structures and stabilities of ionized (9-ethyl) guanine quadruplexes, *Mohammad Azargun* and Travis Fridgen, Memorial University.
- A complete workflow for achieving high accuracy jultiplexed N-terminomics data using TMT10plex, Julian Saba, Udayanath Aich, Rosa Viner, Xiaodong Liu, Srinivasa Rao, Jeff Rohrer, Andreas Huhmer and Chris Pohl, presented by *Michael Blank*, Thermo Fisher Scientific.
- Recent advances and applications in differential mobility spectrometry, *J. Larry Campbell*¹, Yves Le Blanc¹, Chang Liu¹, Bradley Schneider¹ and W. Scott Hopkins², ¹AB Sciex, ²University of Waterloo.
- Use of Triple quadrupole GCMSMS as a confirmatory method for PCDD/Fs, Cristian Cojocariu¹, Manela Abalos², Esteban Abad Holgado² and Paul Silcock¹, presented by *Dwain Cardona*, ¹Thermo Fisher Scientific, Cheshire, UK, ²Spanish Council for Scientific Research (CSIC), Institute of Environmental Assessment and Water Research, Barcelona, Spain.
- Q-ToF instrument for studies of intact non-covalent complexes under native conditions, Willemijn van der Laan, *Jan Commandeur*, Jerre van der Horst and Nico Wortel, MS Vision.

- Analysis by high-resolution mass spectrometry (FT-MS) of *Aspergillus niger* overproducing putative transcription regulators of secondary metabolic pathways, *Jean-Pierre Falgueyret*, Annie Bellemare, Marianne Desautels, Marcos Di Falco, Nadeeza Ishmael, Sandrine Marqueteau, Marie-Claude Moisan, Sylvester Palys, Josée Vandal and Adrian Tsang, Centre for Structural and Functional Genomics, Concordia University.
- Characterization of an improved QTOF for proteomics, M. Lubeck, S. Kaspar, A. Michalski, O. Raether, C. Gebhardt and C. Baessmann, presented by *Jim Kapron*, Bruker Ltd.
- Targeted MS analysis of urine metabolites differentially expressed in asthma patients, *M. M. Khamis*¹, H. Awad¹, D. J. Adamko², L. Li³, R. Zhou³ and A. El-Aneed¹, ¹College of Pharmacy and Nutrition, University of Saskatchewan, SK, , Canada, ²Department of Pediatrics, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada, ³Department of Chemistry, University of Alberta, Edmonton, AB, Canada.
- Chromatographic behaviour of peptides containing oxidized methionine residues in proteomic LC-MS experiments: complex tale of a simple modification, Ying W. Lao, Dmitry Shamshurin, Vic Spicer and *Oleg V. Krokhin*, University of Manitoba, Winnipeg, Canada
- Identification and quantification of ceramides and glucosylceramides in cellular extracts using LC-ESI-MS/MS method, *Si Mi* and Jonathan M. Curtis, University of Alberta.
- The analysis of folates in pulse crops by LC-MS/MS, *Randy W. Purves*¹, Ashokkumar Kaliyaperumal¹, Stephen J. Ambrose², Ambuj B. Jha¹, Marwan Diapari¹, Haixia Zhang², Kirstin E. Bett¹, Bunyamin Tar'an¹, Thomas D. Warkentin¹ and Albert Vandenberg¹, ¹University of Saskatchewan, ²National Research Council.
- Analysis of post-translational modifications of histones in *Fusarium graminearum*, Nadia Ponts, Slavica Djuric-Ciganovic and *Christof Rampitsch*, Agriculture and Agrifood, Canada.
- Developing a middle-down method for integrative structural proteomics, *Dave Schriemer*, University of Calgary.
- A novel hybrid SFC/UHPLC/MS system optimized for low peak dispersion, *Jean-Francois Roy*, Patric Hoerth, Rick Wikfors and Tom Van de Goor, Agilent Technologies.
- Mass spectrometry-based phospholipidomics of oncolytic virus-infected chronic myelogenous leukemia cells, Michael Atkins¹, Carlos Canez¹, Julia Hajjar², Geeta Waghray², Harold Atkins² and *Jeffrey C. Smith*¹, ¹Institute of Biochemistry and Department of Chemistry, Carleton University, Ottawa, Canada, ²Centre for Innovative Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, Canada.
- Structure and Dynamics of FoF1-ATP synthase probed by HX-MS, *Siavash Vahidi*, University of Western Ontario.
- Tandem mass spectrometric analysis of a series of chlorogenic acid isomers, *Jamie Willems*¹, W. Mohammed-Saeid², M. Khamis², G. Katselis³, N. Low¹ and A. El-Aneed², ¹Department of Food and Bioproduct Sciences, ²College of Pharmacy and Nutrition, ³Department of Medicine, University of Saskatchewan.

Friday, December 5, 2014

Mechanisms and Methods Chair: Lars Konermann

- 8:00 Shining light on the dissociation of PAH ions, *Paul M. Mayer*, University of Ottawa.
- 8:20 Radical peptide ions, K. W. Michael Siu, University of Windsor.
- 8:40 Structures and stabilities of ionized (9-ethyl) guanine tetraplexes, *Mohammad Azargun* and Travis D. Fridgen, Memorial University, St. John's.
- 9:00 Understanding (or not) extractive electrospray using tandem mass spectrometry, *Gary Glish*, University of North Carolina, Chapel Hill.
- 9:20 A rapid method for structural identification of N-glycans, *Ting Song* (Winner of a Lake Louise 'All Sponsor' Travel Award), University of California, Davis.
- 9:40 Bio-solid phase extraction/tandem mass spectrometry, *John Brennan*, McMaster University, Hamilton.
- 10:00 Discussion

 Coffee Break

Environmental and Biological Applications

- 10:30 LC-MS studies of sweeteners: effects on human health and environment, *Xing-Fang Li*, University of Alberta, Edmonton.
- Tandem mass spectrometry uncovers chlorination reaction pathway for X-ray contrast media in drinking water treatment, *Susan Richardson*, University of South Carolina, Columbia.
- 11:10 Structural mass spectrometry for the analysis of complex samples in systems, synthetic, and chemical biology, *John A. Mclean*, Vanderbilt University, Nashville.
- Progress in human secretome analysis with biomedical relevance, *Peter Verhaert*, Delft University of Technology.
- 11:50 Discussion
- 12:00 Lunch
- 13:30 Geology of Lake Louise, with Bob Davidson, in lobby
- 14:00 Informative walk up the lake with Bob Davidson
- 18:00 Cocktails Victoria Ballroom
- 19:00 Banquet Victoria Ballroom

Saturday, Dec. 6, 2014

Peptides, Proteins and Protein Modifications Chair: Lars Konermann

- 8:00 Recent trends in antibody-drug conjugate (ADC) bioanalysis & biotransformation, *Fabio Garofolo*, Algorithme Pharma.
- 8:20 Qualitative and quantitative analysis of NAPQ1 protein adducts by LC-MS/MS, *Lekha Sleno*, Université du Québec à Montréal.
- 8:40 Mass spectrometry for the study of protein methylation, *Daniel Figeys*, University of Ottawa.
- 9:00 Proteomic LC-MS/MS lessons in peptide chromatography: which amino acid is the most hydrophobic?, *Oleg Krokhin*, University of Manitoba, Winnipeg.
- 9:20 Towards using coarse-grained and atomistic simulations to aid the interpretation of mass spec data, *Peter Tieleman*, University of Calgary.
- 9:40 Discussion
 Coffee Break

Protein Interactions and Hydrogen/Deuterium Exchange Chair: David Schriemer

- 10:10 Tandem mass spectrometry applications on an Orbitrap with extended mass range, *Albert Heck*, Utrecht University.
- 10:30 Discovery and characterization of ligands for human noroviruses, *Ling H*an (CSMS Travel Award Winner, sponsored by Thermo Fisher Scientific), University of Alberta, Edmonton.
- 10:50 Challenges and solutions for SWATH-HXMS², *Kyle Burns*, University of Calgary.
- 11:10 Protein-ligand interactions studied by hydrogen exchange mass spectrometry, *Modupeola Sowole* (CSMS Travel Award Winner, sponsored by Waters), University of Western Ontario, London.
- 11:30 Allosteric changes in STAT3 upon complexation with drug candidates, *Derek Wilson*, York University, Toronto.
- Effects of salt adducts on the dissociation behavior of electrosprayed protein complexes, *Lars Konermann*, University of Western Ontario, London.

- 12:10 Discussion
- 12:15 Lunch

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