

LAKE LOUISE XVIII

18th Workshop on Tandem Mass Spectrometry

Thursday, December 1, 2005, Morning Session

Chair: Simon Gaskell

- 8:30 Introductory Remarks: Gary Glish
- 8:40 Data Mining Strategies for Phosphoproteome : Analyses of complex cellular extracts, *Pierre Thibault*, U. Montreal
- 9:25 Mapping of phosphorylation sites with low-specificity proteases, *Andreas Schlosser*¹, Jens T. Vanselow², Achim Kramer², Institute of Medical Immunology, Charité, Berlin, ¹Mass Spectrometry Lab, ²Chronobiology Lab
- 9:45 Accurate mass mapping and sequencing of corpus cardiacum neuropeptides by means of MALDI-*oa*TOF MS/MS and UPLC-*oa*TOF MS/MS, *Peter Verhaert*¹, Gerold Schwarz², Art Kroon¹, Laetitia Cravello², Hans Vissers², ¹Delft U. Technology, ²Waters

10:05 Discussion

10:10 Break

- 10:35 Identification and structural analysis of methylglyoxal-insulin adducts using MALDI-TOF MS and Q-TOF LC-MS/MS, *Andrew Ross*, Doug Olson, Xuming Jia, Lingyun Wu, NRC
- 10:55 Studying molecular mechanisms of mouse brain plasticity during development and adulthood: a proteomic approach, *B. Van de Plas*, G. Van den Bergh, S. Clerens, L. Arckens, P. Verhaert, U. Leuven
- 11:15 Toxicity-Based Identification of Drinking Water Disinfection By-Products Using ESI-MS and ESI-MS/MS, *Susan D. Richardson*¹, F. Gene Crumley¹, Junghoon Choi¹, Michael J. Plewa², Elizabeth D. Wagner², Todd H. Mize³, Ron Orlando³, Richard N. Winn³, Leah Williamson³, Michael Bartlett³, ¹U.S. EPA, ²U. Illinois, ³U. Georgia
- 11:35 A Study of Flavonoid Glycosides Using Mass and Nuclear Magnetic Resonance Spectroscopies Combined with *ab initio* Chemical Computation, *Raymond E. March*, Errol G. Lewars, Darcy C. Burns, David A. Ellis, Trent U.

11:55 Discussion

12:00 Lunch

Afternoon Session

Chair: Gary Glish

- 14:00 Probing ions from simple aromatic molecules by reactivity and by spectroscopy, *Simonetta Fornarini*, U. Rome
- 14:45 Competing rearrangement reactions in small gas-phase ionic complexes: The internal SN2 and nitro-nitrite rearrangements in nitroalkane proton-bound pairs, *Paul Mayer*, U. Ottawa
- 15:05 Multiplexed Peptide Modification Analysis by Stepped Parallel CID, Ion Trapping, and Data Processing, Michael D. Hoffman¹, Matthew J. Sniatynski¹, Jason C. Rogalski¹, J.C. Yves LeBlanc², *Juergen Kast*¹, ¹British Columbia, ²MDS Sciex

15:25 Analysis of the Success Rate of Various Modes of MS/MS Analysis in Identifying Proteins from Peptides using LTQ-FTMS and Q-TOF Systems, *Terry Cyr*, Health Canada

15:45 Discussion

15:50 Break

16:10 Structure elucidation of oligosaccharides by CID and IRMPD, *Carlito Lebrilla*, U. California, Davis

16:55 High Amplitude Short Time Excitation CID using Heavy Gases, *Connell Cunningham, Jr.*, Gary L. Glish, U. North Carolina

17:15 Metabolite ID using LC/QqTOFMS with collision energy switching - Getting the most out of your first run, *Mark Wrona*, Merck Frosst

17:35 Discussion

18:00 Dinner

Evening Session

Chair: Paul D'Agostino

20:00 An examination of mechanisms in Dopant Enhanced - Atmospheric Pressure PhotoIonization or rather PhotoInduced Chemical Ionization, *Rob O'Brien*, Krista Gaebel, Okanagan Regional Chemical Analysis Centre

20:20 Biomarker Discovery in Human Cerebral Spinal Fluid for Neurodegenerative Disease, *Fadi A Abdi*, C. Pan, J. Quinn, E. Peskind, J. Jankovic, J. Nutt, K. Chung, J. Leverenz, A. Samii, M. McIntosh, J. Jin, Y. Wang, J. Li, T. Montine, and J. Zhang, Applied Biosystems

20:40 Ultra-Low Volume Fraction Collection from NanoLC Columns for Improved Mass Spectrometric Analysis of Protein Phosphorylation and Glycosylation, *Colleen K. Van Pelt*, Thomas N. Corso, Jie Li, Celeste Ptak, Xian Huang, Advion BioSystems

21:00 Discussion

21:05 Poster Session

An Investigation of Chlorotetracycline Epimerization Using LC-MS/MS, *Jonathan Bailey, Kerry M. Peru*, Allan J. Cessna, and *John V. Headley*, National Water Research Institute

HPLC-chip/MSMS mass spectrometry compared to Nano-LC/MSMS mass spectrometry for metabolite identification, *Linda Côté*, Anabel Fandiño, Edgar Nägele, Agilent Technologies

Biomarkers for Fabry Disease: the importance of LC/MS/MS, *Denis Cyr*, Christiane Auray-Blais, Robert Giguère, Bernard Lemieux, U. Sherbrooke

Desorption Electrospray Tandem Mass Spectrometry (DESI-MS/MS) of Solid Phase Microextraction (SPME) Fibres, *Paul A. D'Agostino*, Carmela R. Jackson Lepage, James R. Hancock, Claude L. Chenier, Adam D. Morcom, DRDC Suffield

Off-line 2D LC Approaches for the Analysis of Intact Proteins followed by Proteolytic Digestion and LC/MS/MS Analysis, *Mark van Gils*¹, Irina Dragan², Bas Dolman², Evert-Jan Sneekes² and Remco Swart², ¹Dionex Corporation, ²LC Packings

Multiple Losses of Neutral C14H14 in the MS/MS of Several Perbenzylether Intermediates in the Synthesis of Green Tea Constituents, A Lesimple, M Di falco, Y Richard, S Lesimple, Z Wang, T- H Chan, *O A Mamer*, McGill U.

Fluorescence from ino-target gas collisions, Clement Poon and *Paul Mayer*, U. Ottawa

Analysis of lincomycin and spectinomycin in ground water and surface runoff from manure treated fields, S.L. Kuchta, A.J. Cessna, *K.M. Peru*, *J.V. Headley*, National Water Research Institute

Analysis of supramolecular complexes between tannins and peptides by MS/MS, Benoît Plet, *Jean-Marie Schmitter*, Institut Européen de Chimie et Biologie

Statistical distribution of deuterium incorporation offers insights on the deuterium scrambling phenomenon, John Chik, *Dave Schriemer*, U. Calgary

The Trypsin Turboreactor - an integrated system for real-time sub-nanogram protein identification, Gordon Slysz, *Dave Schriemer*, U. Calgary

MALDI MS/MS investigation of organic semiconductor molecules, *Svitlana V. Shcherbyna*¹, Diethard K. Bohme¹, Vladimir I. Baranov², Alexander Loboda², ¹York U., ²MDS Sciex

Structural Elucidation of Rapamycin Degradents in Solution Using a Linear Ion Trap and Predictive Software: Using MSn to Simplify Compound Identification, *Mark Szeew*, Mary Blackburn, Thermo Electron

Determination of Algal Toxins in Surface and Treated Waters by Solid Phase Extraction and Liquid Chromatography - Tandem Mass Spectrometry (LC-MS/MS), S. Jenkins, J. Newman, *M.A. Trikoupis*, V.Y. Taguchi, Ministry of the Environment

Friday, Dec. 2, Morning Session

Chair: Orval Mamer

8:45 Proteomics-grade de novo sequencing of peptides using complementary fragmentation techniques and high mass accuracy of FT ICR MS., *Roman Zubarev*, Uppsala U.

9:30 Strategies for the fractionation and identification of complex mixtures of proteins and peptides using continuous Free-Flow Electrophoresis (FFE) coupled to RP-HPLC and LC-ESI-MS/MS, *Robert L. Moritz*, Hong Ji, Frederic Schutz, Lisa M. Connolly, Eugene A. Kapp, Terence P. Speed, Richard J. Simpson, Ludwig Institute for Cancer Research, The Walter and Eliza Hall Institute of Medical Research, U.California, Berkeley

9:50 Identification of Copper-binding Plant Proteins Using LC-MS/MS., *Cory Sonntag*, Andrew Ross, NRC

10:10 Discussion

10:15 Break

- 10:35 Quantitative Proteomics Based on LC-MALDI MS and MS/MS, *Liang Li*, U. Alberta
10:55 Isotope-Coded Protein Labeling: A New Strategy for Multiplexed Relative Protein Quantitation, *Gary H. Kruppa*, Detlev Suckau, Bruker Daltonics
11:15 Multiple MS and tandem MS strategies for the characterisation of cross-linked proteins, Dalila Bensaddek, *Simon J Gaskell*, U. Manchester
11:35 Top Down Mass Spectrometry of Large (200 kDa) Proteins, *Xuemei Han*, Mi Jin, Kathrin Breuker, Fred McLafferty, Cornell U.

11:55 Discussion

12:00 Lunch

- 13:30 Information walk, with Bob Davidson, up lake
16:30 Broomball, Canada v. The World
18:30 Banquet

Sat., Dec. 3, Morning Session

Chair: Paul Mayer

- 8:45 Newer Mass Spectrometry-Based Instrumentation for Protein Characterization, *K.W. Michael Siu*, York. U.
9:30 The Ion Conveyor: Development and Applications of an Ion Source Incorporating an Electrodynamic Focusing Device, *Mark P. Barrow*¹, Alex W. Colburn¹, Matthew C. Gill¹, Anastassios E. Giannakopoulos¹, Peter J. Derrick¹, John V. Headley², Kerry M. Peru², ¹U. Warwick, ²National Water Research Institute
9:50 12T-FTICR-MS for proteomics and metabolomics, *Christoph Borchers*, U. North Carolina

10:10 Discussion

10:15 Break

- 10:35 MS/MS Performance Factors of Triple Quadrupole and Q-ToF Mass Spectrometers using an Axial Potential Gradient Acceleration Collision Cell, *John Fjeldsted*, Agilent Technologies
10:55 Tandem mass spectrometry using LTQ Orbitrap hybrid mass spectrometer, *A.A.Makarov*, K. Strupat, S. Horning, E. Denisov, A. Kholomeev, W. Balschun, O. Lange, Thermo Electron
11:15 Enhanced oa-TOF mass spectrometry by coupling to Ion Mobility, *Thérèse McKenna*, Jason L. Wildgoose, Steven D. Pringle, Kevin Giles and Robert H. Bateman, Waters
11:35 Increasing Peptide Fragmentation in a Quadrupole Ion Trap: Does it Help Identify Unknowns?, *Gary Glish*, U. North Carolina

11:55 Discussion

12:00 Adjourn and Lunch

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