LAKE LOUISE XV

15th Workshop on Tandem Mass Spectrometry

Thursday, December 5, 2002

Chair: Simon Gaskell

8:05 Introductory Remarks, Gary Glish

8:15 Ion-molecule reactions: What can they tell us about the gas-phase structure of divalent metal complexes, ***Richard W. Vachet***, U. Massachusetts

8:55 Reactions of the Phenylnitrenium Ion in the Gas Phase: Observing Electrophilic Reactivity Leading to Carcinogenic Activity, ***J.Larry Campbell***, Hilkka I. Kenttämaa, Purdue U.

9:15 New Applications, Fragmentations, and Mechanisms in Electron Capture Dissociation Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ECD-FT-ICR-MS), ***Robert Hudgins***, York U.

9:35 Tandem AMF-ESA-FTICR Studies of Mechanisms in Surface-Induced Dissociation, ***JeanH. Futrell***, Pacific Northwest National Laboratory

9:55 Discussion

10:00 Break

10:20 Charge Separation and it's applications on a hybrid QqTOF Mass Spectrometer, ***Igor Chernushevich***, MDS Sciex

10:40 Rapid, Accurate FT-ICR MS/MS, Greg T. Blakeney, Michael J. Chalmers, ***Mark R. Emmett***, Kristina Hakansson, Christopher L. Hendrickson, Melinda A. McFarl, John P. Quinn, Alan G. Marshall, Florida State U.

11:00 Orthogonal-injection MALDI TOF MS and MS/MS with a high repetition rate laser, ***Werner Ens***, Maciej Bromirski, Natalia Bykova, Alexander Loboda, Ken Standing U. Manitoba

11:20 A new AP-Maldi Source coupled to an Ion Trap Mass Spectrometer, ***Alex Mordehai***, Agilent Technologies

11:40 MS/MS scans using a hybrid Quadrupole-Linear Ion Trap Mass Spectrometer, ***James Hager***, MDS Sciex

12:00 Discussion

12:10 Break for Lunch

Chair: Gary Glish

14:00 The tandem mass spectrometer as chemical reactor: From N4 to polyvinylacetate, ***Paul M. Mayer***, U. Ottawa

14:45 Fragmentation of the b2 and a2 Ions in Protonated GGX, GAX, and AGX: A Mechanistic Evaluation Using Density Functional Theory and Threshold Collision-Induced Dissociation, ***Houssain El Aribi***, C. F. Rodriquez, A. C. Hopkinson, K. W. Michael Siu, York U.

15:05 Isomerization in Gas Phase Ions, ***Terry McMahon***, U Waterloo

15:25 Discussion

15:30 Break

15:50 Barrier Height Tritration for Keto-Enol Tautomerization by Photoionization Combined with Chemical Monitoring, ***Helmut Schwarz,*** Technical Institute of Berlin

16:30 Tandem Mass Spectrometry of Doubly and Triply Charged Solvated Metal Complexes, S. Patel, A. C. Hopkinson, ***K. W. Michael Siu***, York U.

16:50 ICP/SIFT Tandem Mass-Spectrometer Studies of Reactions of Metal Ions with Nitric Oxide, ***Diethard K. Bohme***, York U.

17:30 Discussion

Chair: Paul D'Agostino

20:00 Desorption/Ionization on Silicon (DIOS), ***Gary Siuzdak***, Scripps Research Institute

20:40 New Development in MALDI Sample Preparation for Proteomics Applications, ***Liang Li***, U. Alberta

21:00 Discussion

21:10 Poster Session

Posters

Gas-Phase Kinetic Measurements of Metal-Ion Adducts M(pyrrole)1,2+ (M = Cu, Ni) with Biological Gases, ***Michael Jarvis***, York U.

Reactions of Metal Ion Adducts of 1-methyl-imidazole with Biological Gases, ***Voislav Blagojevic***, York U.

Computational Approaches to Optimized Peptide Sequencing, ***Juergen Kast***, U. British Columbia

LC-ESI-MS and GC-MS Analysis of a Synthetic Tabun Sample, ***Paul A. D'Agostino***, Claude L. Chenier, James R. Hancock, DRDC

Triple-quadrupole like MS/MS spectra of azaspiracids by wide-range activated CID on a commercial ion trap instrument, ***Stephan Brombacher***, NRC Institute of Marine Biosciences

Identifying Brassica Napus Root Exudate Proteins by De Novo Sequencing, ***Randy M. Whittal***, Urmila Basu, Gregory J. Taylor, U. Alberta

Separation and Detection of Ephedrine Derivates in Natural Health Products by Flow Injection - Electrospray Ionization - High Field Asymmetric Waveform Ion Mobility Spectrometry - Mass Spectrometry, Margaret A. McCooeye, Luyi Ding, ***Zoltan Mester***, National Research Council

Speciation and Characterization of Dissolved Metal-Binding Peptides using Electrospray MS and MS/MS, Sarah L. Luettgen[1], Steve J. Ambrose[2], ***Doug J.H. Olson***[2], Andrew R.S. Ross[2], [1]U. Victoria, [2]National Research Council

1D and 2D LC/MS/MS Using a Nanoflow LC/MS/MS Ion Trap, ***Linda Cote***, Agilent Technologies

Peptide Mapping Using an Optimized Microflow ESI Nebulizer, ***Linda Cote***, Agilent Technologies

Detection of phosphorylated peptide by HPLC under alkaline pH, François Lépine[1], ***Daniel Boismenu***[2], Souad Lesimple[2], Alexander Bell[2], John Bergeron[2], Orval Mamer[3], [1] INRS Institut

Armand-Frappier, [2]Montréal Network for Pharmaco-Proteomics and Structural Genomics, McGill University, [3]McGill University Mass Spectrometry Unit

Applications of LC/MS to the Study of the Toxicity Characteristic Leaching Procedure, ***Anna Trikoupis***, Ontario Ministry of Environment and Energy

High Sensitivity and Resolving Power for a Zspray/FTMS for Proteomics, ***Robert T. McIver***, IonSpect

Matrix and Ion Suppression Effects in Tandem Mass Spectrometry, ***Lawrence Hogge***, T.Gurnsey, S. Johnson, ***Gord McKay,*** Pharmalytics

The Fragmentation of the Cluster Ion Including HC1: $(M1+HCl+M2+H)^+$ (M1,M2=Amines) – Proton Affinities of Drugs of Abuse, ***Kimio Isa*** (Fukui U.), Hideyuki Takezwa (Fukui U.), Shigeki Matumura (Forensic Science Lab., Fukui Prefectural Police H. Q.)

Friday, December 6, 2002

Chair: Gord McKay

8:45 Structure and stability of non-covalent protein complexes in the gas phase, ***John. Klassen***, U. Alberta

9:25 Effect of Buffer Cations and of H3O+, on the Charge States of Native Proteins Obtained by ESIMS and the Significance of Findings to Bioanalytical Applications, Udo Verkerk, Michael Peschke, ***Paul Kebarle***, U. Alberta

9:45 Recent Advances in De Novo Sequencing using a Tandem TOF, ***Alfred. Yergey***, NIH

10:05 Discussion

10:10 Break

10:30 Structural Elucidation of Biological Molecules using a MALDI QIT TOF MS, ***Rachel L. Martin***, Emmanuel Raptakis, Shaukat Bekar, Shimadzu Biotech

10:50 MALDI-MS/MS and MALDI-""pseudo""-MS3 for protein characterization and protein chip technology, Christina S. Raska, Carol E. Parker, Zbigniew Dominski, William F. Marzluff, Susan W. Sunnarborg, David C. Lee, Marshall Pope, Cai Huang, Jun Han, Gary L. Glish, ***Christoph H. Borchers***, U. North Carolina

11:10 A study of peptide conformation and fragmentation using energy resolved mass spectrometry, ***Shabaz Mohammed***, Simon J. Gaskell, UMIST

11:30 Structural Analysis of Protonated Dipeptide Ions by CID Spectra, M. Gotou, ***Kimio Isa***, R. Nakata, Fukui U., N. Kobayashi, Nicca Chemical Co. Ltd.

11:50 Discussion

11:55 Break for Lunch

18:30 Workshop Banquet

Saturday, December 7, 2002

Chair: Orval Mamer

9:00 Identification of Gas and Particle Products using Tandem MS, ***Christine Dalton***, Mohammed Jaoui, Richaard M. Kamens, Gary L. Glish, U. North Carolina

9:20 LC/MS/MS of Tetracycline photolysis in two prairie waters Under natural sunlight conditions, ***Brij Verma*** [1,2], John V. Headley [1]*, Kerry M. Peru [1], Richard D. Robarts [1],

Nick Christofi [2], [1]National Water Research Institute, [2]Napier U

9:40 Optimization of Ion Trap Data-Dependent MS/MS Acquisition Parameters for Proteomics, ***Brett R. Wenner***, Bert C. Lynn, U. Kentucky

10:00 Discussion

10:05 Break

10:25 Sequencing Synthetic Copolymers using Electrospray Ionization Mass Spectrometry, ***Mraie-Soleil Giguère***, Marc Dubé, Paul Mayer, U. Ottawa

10:45 High Performance Quantitation and Metabolite Identification on a High-Resolution Triple Quadrupole Mass Spectrometer, ***Kevin J. McHale***, Witold Winnik, Joseph J. Mulholland, Maurizio Splendore, Gary Paul, Thermo Finnigan

11:05 Clinical Mass Spectrometry:From the Cradle to the Grave, ***Scott Gillingwater***, Micromass

11:25 It's Warmer in North Carolina: Improving MS/MS using Heat, ***Gary Glish***, U North Carolina

11:45 Discussion & Closing Remarks

Lunch

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