

LAKE LOUISE IX
The Ninth Lake Louise Workshop on Tandem Mass Spectrometry
All meetings to be held in the Tom Wilson Room on the 7th Floor

Thursday 5th December

8.30 Welcome and Announcements

ION TRAPPING (Bob Boyd, Chair)

8.35 **Alan Marshall** (Florida State University, Tallahassee, Florida): Tools for determination of biological macromolecular structure.

9.20 **Frank Laukien, J.P. Speir, J. Wronka, G.H. Kruppa and T. Zhang** (Bruker Instruments, Billerica, Massachusetts): Correlated sweep parent ion isolation and quasi-internal calibration for fast, reliable FT MS/MS experiments.

9.40 **Discussion**

9.55 **Poster viewing and coffee**

10.45 **Gary Glish** (University of North Carolina, Chapel Hill, North Carolina): Effects of time and energy in MS/MS using a quadrupole ion trap.

11.30 **Ray March** (Trent University, Peterborough, Ontario): A simulation study of ion kinetic energy variation during resonant excitation in a stretched quadrupole ion trap.

11.50 **Discussion**

12.00 **Lunch**

ANALYSIS OF BIOMOLECULES (Simon Gaskell, Chair)

13.30 **Jane Thomas-Oates** (University of Utrecht, The Netherlands): Tandem MS in the study of host-symbiont interactions: achievements and pitfalls.

14.15 **Pierre Thibault** (National Research Council, Ottawa): Probing sialic acid glycoproteins and oligosaccharides from antigenic bacteria.

14.35 **Joseph Banoub** (Department of Fisheries and Oceans, St Johns, Newfoundland): Electrospray tandem mass spectrometry of carbohydrate amphipathic molecules.

14.55 **John S. Klassen and Paul Kebarle** (University of Alberta, Edmonton): CID threshold energies of protonated glycine, Gly₂ and Gly₃, and mechanism of formation of b, a, and y ions.

15.15 **Discussion**

15.30 **Coffee**

- 15.35 **Lars Konersmann** and Don Douglas (University of British Columbia): Protein folding studied by time-resolved ES-MS.
- 15.55 Scott G. Summerfield and **Simon Gaskell** (UMIST, Manchester, UK): Peptide ion fragmentation as a function of stereochemistry.
- 16.15 **Mark Bolgar** (Bristol-Myers Squibb, New Brunswick, New Jersey) and Simon Gaskell (UMIST, Manchester, UK): Tandem MS evidence for lipid/protein conjugation in oxidized low density lipoprotein.
- 16.35 **Ad de Jong** (National Institute of Public Health and Environment, Bilthoven, The Netherlands): Analysis of MHC Class I associated peptides (antigens) by micro-LC-MS/MS.
- 16.55 **Bill Davidson** (Sciex, Thornhill, Ontario): Applications of triple quadrupole MS/MS to proteome characterization and to neonatal screening.
- 17.15 **Discussion**
- 18.00 **Dinner**

PHARMACEUTICAL APPLICATIONS (Gordon McKay, Chair)

- 20.00 **Paul Pearson** (Pharmacia-Upjohn, Kalamazoo, Michigan): Enzymes, isotopes and mass spectrometry: applications of mass spectrometry in drug metabolism.
- 20.45 **Timothy Olah** (Merck, West Point, Pennsylvania): The use of LC-MS/MS for multiple analyte pharmacokinetic studies in drug discovery.
- 21.05 **Daniel Boismenu**, Orval Mamer, Line Ste-Marie, Luc Vachon and Jane Montgomery (McGill University, Montreal, Quebec): *In vivo* hydroxylation of the neurotoxin, 1-methyl-4-phenylpyridinium, and the effect of monoamine oxidase inhibitors: electrospray MS-MS analysis of intra-striatal microdialysates.
- 21.25 **Rod Mathews** (Pharmacia-Upjohn, Kalamazoo, Michigan): Probing the interaction of nitric oxide with biological targets using mass spectrometry.
- 21.45 **Jack Cunniff** (Finnigan, San Jose, California): LCQ: a revolutionary benchtop LC-MSⁿ instrument.

Friday 6th December

INSTRUMENTATION AND MECHANISMS (Gary Glish, Chair)

- 8.30 **Vicki Wysocki** (University of Arizona, Tucson, Arizona): Surface-induced dissociation: an effective activation method for tandem mass spectrometry.
- 9.15 **Paul Danis** (PerSeptive Biosystems, Framingham, Massachusetts): Peptide sequencing update: PSD and CID experiments with a new MALDI-TOF instrument.

9.35 **Bob Bordoli** (Micromass UK Ltd., Manchester, UK): Q-ToF: a novel tandem quadrupole-orthogonal acceleration time-of-flight MS and MS/MS instrument.

9.55 **Discussion**

10.15 **Coffee**

10.35 **Chris Enke** (University of New Mexico, Albuquerque): Implementation of photo-induced dissociation in tandem time-of-flight mass spectrometry.

11.20 **Jonathan Curtis** (National Research Council, Halifax, Nova Scotia): MS and MS/MS applications of the DEPHY Technologies metastable atom bombardment ion source.

11.40 **Michel Bertrand** and **Dennis Faubert** (University of Montreal, Quebec): Metastable atom bombardment as an ion source for analytical mass spectrometry.

12.00 **Discussion**

12.15 **Lunch**

Afternoon free

19.30 for

20.00 **Workshop Dinner**

Saturday 7th December

APPLICATIONS TO STRUCTURAL CHARACTERIZATION AND MIXTURE ANALYSIS (**Pierre Thibault**, Chair)

8.30 **Julie Leary** (University of California, Berkeley, California): Stereochemical differentiation of bio-inorganic complexes using ESI tandem mass spectrometry.

8.50 **K.W.M. Siu** (National Research Council Institute for National Measurement Standards, Ottawa): Structure of silver-containing adducts of electrospray-generated proteins and peptides.

9.10 **Andrew Kutchinsky**, **Igor Chernushevich**, **Werner Ens**, **Ken Standing**, **Ayeda Ayed** and **Harry Duckworth** (University of Manitoba, Winnipeg): The application of ESI/TOF mass spectrometry in the study of noncovalent complexes of citrate synthase and NADH.

9.30 **Magda Claeys**, **L. Nizigiyimana**, **H. Van den Heuvel** (University of Antwerp, Belgium) and **P.J. Derrick** (University of Warwick, Coventry, UK): Mechanistic aspects of charge-remote fragmentation in saturated and mono-unsaturated fatty acid derivatives; evidence for homolytic cleavage.

9.50 **Discussion**

10.10 Coffee

10.30 **Anna Smirnov** et al. (Department of Earth Sciences, Memorial University, Newfoundland): Molecular and isotope chemistry of PAHs in the sediments of Lake Erie.

10.50 **Jim Scrivens** (ICI, Wilton, UK): Characterization of oligomeric systems using MALDI MS/MS.

11.10 **Frank Benoit** and Cariton Kubwabo (Environmental Health Directorate, Ottawa): Electrospray MS/MS of sulphonated azo dyes.

11.30 **Bob Boyd** (National Research Council, Halifax, Nova Scotia): An MS/MS investigation of competition between charge site-remote and mixed-site fragmentation of long-chain quaternary ammonium ions.

11.50 Discussion

12.00 Close of Workshop

POSTERS

Paul D'Agostino, James R. Hancock and Lionel R. Provost. (DRES, Suffield, Alberta): Mass spectrometric profiling of bacterial phospholipids.

Daniel Boismenu, Francois Lepine and Orval Mamer (McGill University, Montreal, Quebec): Collision-induced oxygen addition to phthalate esters.

John Patterson et al. (Agriculture Canada, Saskatoon, Saskatchewan): Confirmation of veterinary drug residues in tissue by API-LC/MS/MS.

John Headley et al. (National Hydrology Research Institute, Saskatoon, Saskatchewan): Tandem MS of explosives in soil and groundwater samples.

L. Nizigiyimana, H. Van den Heuvel and **Magda Claeys** (University of Antwerp, Belgium): Comparison of low- and high-energy collision-induced dissociation tandem mass spectrometry in the analysis of ricinoleic acid and ricinelaic acid.

Bob Bordoli (Micromass UK, Manchester, UK): Fast switching between MS and MS/MS on a tandem magnetic sector-TOF instrument.

D. Grant and **Leo Milward** (Agriculture Canada, Calgary): MS/MS confirmation of flumprop-methyl residues in silage extracts.

A.N. Krutchinsky, I.V. Chernushevitch, V.L. Spicer, W. Ens and **Ken Standing** (University of Manitoba, Winnipeg): Flight-time distributions for ions passing through an RF quadrupole ion guide at a pressure of ca. 0.1 torr.