

LAKE LOUISE IV

The Fourth Annual Lake Louise Workshop on Tandem Mass Spectrometry 21 November - 23 November, 1991

All Meetings are to be held in the Tom Wilson Room on the 7th Floor

Thursday, 21 November

8:30 Welcome and announcements

TANDEM MASS SPECTROMETRY USING ION TRAPS (Gary Glish, Chair)

8:35 GARY GLISH, K.J. Hart, S.A. McLuckey (Oak Ridge National Laboratory), M.J. Charles: Fundamentals of MS/MS in an ion trap: Part I

9:00 M. JUDI CHARLES, S.A. McLuckey, G.L. Glish (Oak Ridge National Laboratory): Fundamentals of MS/MS in an ion trap: Part II

9:25 JODIE JOHNSON (University of Florida), R.A. Yost and N. Yates: Practical MS/MS on a quadrupole ion trap: potentials and challenges

9:45 Discussion

10:00 Coffee

10:30 JAE C. SCHWARTZ (Finnigan): ITMS tandem MS for peptide sequencing: strengths and weaknesses

11:00 STEVE HOKE, R.G. Cooks (Purdue University): Recent developments in ion trap technology at Purdue.

11:20 RAY E. MARCH (Trent University): Trajectory simulations of trapped, exited and ejected ions in or from the ion trap.

11:40 XIAOMIN WANG (York University): Tandem mass spectrometry on the modified ion trap detector

12:00 Discussion

12:30 Lunch

ENVIRONMENTAL APPLICATIONS (Judi Charles, Chair)

2:00 CHRIS ENKE (Michigan State University): The search for congener specificity through MS/MS

2:40 COLIN MOORE (Kratos): High resolution or hybrid MS/MS?

3:05 COLEEN ROSTAD (US Geological Survey): Selected environmental applications of tandem MS

3:30 Coffee

3:45 TOM CAIRNS (US Food and Drug Administration): Evolving criteria for confirmation of trace level residues by tandem mass spectrometry

- 4:10 ED FURLONG (US Geological Survey): Application of HPLC-MS/MS to environmental samples
- 4:35 BOB VOYKSNER (Research triangle Institute): Electrospray MS/MS for environmental monitoring generating CAD mass spectra without parent ion isolation
- 5:00 JOHN MONAGHAN (ICI C&P): Screening for sulphonated azo dye stuffs by Tandem Mass Spectrometry
- 5:25 KEITH ROLLINS (ICI Advanced Materials Research Centre): A comparison of LSIMS and FD MS/MC spectra of cationic surfactants
- 5:50 Discussion
- 6:30 Dinner

DISCUSSION SESSION ON TANDEM MS OF FULLERENES (Mark Ross, Chair)

- 8:30 Contributions from MARK ROSS (Naval Research Laboratory; Introduction to the fullerenes; characterization of C₆₀⁺/helium collisions); DIETHARD BOHME (York University; MS/MS studies of helium incorporation in fullerenes); STEVE HOKE (Purdue University; Ion trap and triple quadrupole MS studies of fullerenes and fullerene derivatives).

Friday, 22 November

TANDEM MS OF MULTIPLY CHARGE IONS (Bob Boyd, Chair)

- 8:30 BOB BOYD (NRC, Halifax): Multiply charged ions in mass spectrometry: a brief history
- 8:50 DICK SMITH (Batelle Pacific Northwest Laboratories): Activation and dissociation of multiply charged polypeptides and proteins from electrospray ionization
- 9:30 Discussion
- 10:00 Coffee
- 10:30 PAUL KEBARLE (University of Alberta): Determinations of bond energies: $(M^{++} (H_2O)_n = M^{++} (H_2O)_{n-1} + H_2O$
- 11:00 RONG FENG (NRC, Montreal): Collisionally activated dissociation of multiply charged 150 kDa antibody ions
- 11:20 GARY GLISH (Oak Ridge National Laboratory): MS/MS of multiply charged oligonucleotides
- 11:50 Discussion
- 12:30 Lunch

Extended Break

- 3:30 Coffee

COMBINED CHROMATOGRAPHY/TANDEM MASS SPECTROMETRY (Paul Brooks, Chair)

- 3:45 JODIE JOHNSON (University of Florida): Chromatography and tandem MS
- 4:30 STEVE PLEASANCE (NRC, Halifax): High resolution chromatography techniques in conjunction with on-line tandem MS using atmospheric pressure ionization
- 4:55 BORI SHUSHAN, Tom Covey, Ron Bonner (Sciex): Quantitative aspects of LC-MS/MS using atmospheric pressure ionization
- 5:20 STEFAN KROLIK (VG Analytical/Fisons Instruments): Chromatography with MS/MS: a selection of techniques with applications
- 5:45 PAUL D'AGOSTINO (DRES Suffield): United Nations Chemical Disarmament Round Robin Exercise
- 6:00 PAUL BROOKS (Geological Survey of Canada): Use of MS/MS in organic geochemistry
- 7:30 Cocktails, Sun Room
- 8:00 Dinner, Sun Room

Saturday, 23 November

BIOMEDICAL APPLICATIONS (Simon Gaskell, Chair)

- 8:30 STEVE CARR (SmithKline Beecham): Tandem mass spectrometry in the analysis of covalently modified peptides and proteins
- 9:15 LESTER TAYLOR (Burroughs Wellcome, Inc.): Pharmaceutical applications of MS/MS
- 9:40 TONY MALLET (University of London): Small molecule fragmentation in electrospray
- 10:00 Discussion
- 10:15 Coffee
- 10:45 CHESTER MIROCHA (University of Minnesota): Parent/daughter spectra of fusarochromanone
- 11:05 BRIAN MUSSELMAN (JEOL USA, Inc.), Nancy Jensen and Terry Sumpter (Philip Morris Co.) High resolution parent ion scanning: application to phospholipid analysis
- 11:25 KEN SETCHELL (Children's Hospital Medical Center, Cincinnati): FAB-MS/MS for the detection and characterization of ursodeoxycholic acid sulfate - a simple, rapid and non-invasive test of compliance to oral UDCA therapy
- 11:45 SIMON GASKELL (Baylor College of Medicine): Low energy decompositions of peptide ions: general hypotheses

POSTERS

MARGARET DAVIS (University of Washington): Quantitative analysis of a reactive glutathione conjugate by ion spray tandem mass spectrometry

ROBERT DOYLE (Naval Research Laboratory): Hybrid tandem MS of several new nitramines

COLIN MOORE, Barry Wright (Kratos): High energy fragmentation of peptides on a hybrid instrument