Preliminary Agenda for Mass Spectrometry Training Seminar.

Introduction

- What is Mass spectrometry – a short history
- Why Mass Spectrometry?
- Outline of the Course

Basic Instrumentation

**Ionization techniques**
- Electron Ionization
- MALDI
- Atmospheric Pressure Ionization
  - Electrospray
  - APcI
  - APPI
  - Direct Spray Ionization (Direct Analysis in Real Time: DART)
    - DESI
    - DAPCI
    - JeDI
    - Electrospray Assisted Laser Desorption Ionization

**Ion Transfer**
- Principle
- Sample guide
  - Sample cone
  - Capillary
  - Direct vs Indirect
- Ion guide
  - Stack
  - Electromagnetic: quadrupole/hexapole
  - Collisional cooling
  - “T-Wave”
  - FAIMS

**Mass Analysers**
- Magnetic Analysers
- Quadrupole Analysers
- Ion Trap Analysers
- 3D Ion Traps
- Linear Ion Traps
  - Time of Flight (TOF) Analysers
  - Fourier Transform Ion Cyclotron Resonance Analysers
  - Orbi Trap

**Detectors**

- Principles
  - Active Surfaces
  - Secondary emission
- Different types:
  - Electron Multipliers
  - Photo Multipliers

**Vacuum Systems**

- Vacuum stages in a mass spectrometer
- Vacuum pumping:
  - Rough pumping
  - High vacuum pumping
- Vacuum gauges

**Multistage Mass Spectrometers**

- Tandem Systems
  - Triple Quadrupoles
  - TOF-TOF
- Hybrid Systems
  - Double Focussing Mass Spectrometers (B/E-Hybrids)
  - Quadrupole-TOF
  - Quadrupole – Ion Traps
  - Quadrupole-FTICR
  - Orbitrap-Hybrid

**Sample Inlet Systems**

- Direct Injection
- Online Chromatography: LCMS and LCMS/MS
- Hyphenated Techniques
Interpreting Mass Spectral Data

The Basics of Organic Molecules
- Carbon bonds
- Functional groups
- Electronegativity of N and O.

Ionization Mechanisms
- Electron Ionization: Molecular Ion and Fragments
- Atmospheric Pressure Ionization: Pseudo-molecular Ions

Resolution and Accuracy of Mass Spectrometers
- Calculating resolution
- Resolution of different mass analyzers

Isotopic Abundance
- Isotopic patterns of some relevant elements
- Some handy calculations

Expression of Mass
- Nominal/Mono-isotopic/Average
- The Nitrogen rule

Multiple Charging during Electrospray Ionization
- Macromolecules – proteins
  - Alternative Techniques for Mass-measuring proteins…..
- Multiple charging of small molecules
- Recognizing multiply-charged ions

Fragmentation analysis
- Electron Impact Fragmentation vs. Collision Induced Dissociation
- CID in a Triple Quadrupole
  - In-source dissociation
  - Collision cell dissociation – MS/MS
  - Scan types available during MS/MS
- Structural analysis of proteins
  - Sequencing
  - Investigating Post Transcriptional Modifications
Quantification by MS/MS

- The advantage of MS/MS vs. MS
- Sample Preparation in Short
- The necessity of Chromatography
- The Matrix influence
- Steps during Quantification:
  - Method development
  - Validation
  - Production
  - Data analysis

Some Further Applications ..... 

- Metabolite searching
- Analysis of plant extracts....
- Following a reaction …
- Interesting Adducts and Complexes
- MALDI imaging
- MALDI Triple Quadrupole