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