Mass Spectrometry, Principles and Applications

CHEM 3702, Special Topics-Analytical

Fall 2005

Course Coordinator: Dr. Balasingam Murugaverl (VERL)

Time: 11 to 12 pm, Mondays, Wednesday and Tuesday.

Course Overview:

This course will provide advanced training to those who use or plan to use MS instruments and will give an overview of the capabilities and limitations of these techniques for scientists who are new to mass spectrometry or are considering LC/MS or MALDI/MS. Students will come away from this course with an in-depth knowledge of mass spectrometry and state-of-the-art MS techniques in protein analysis.

Course Requirements:

Attendance - since this is a research oriented course, attendance is critical and a significant portion of the grade will be based on attendance.

Evaluation – Your comprehension of the material covered in the lectures will be tested via three quizzes.

Objectives of this Course

- Obtain an overview of mass spectrometry fundamentals and the operational specifics of most important ionization methods mass analyzers, and sample introduction methods.
- Understand the capabilities and limitations of each type of mass spectrometers for chemical analysis.
- Learn the principles and application of tandem MS and post source decay.
- Mini research projects designed to provide hands on approach to method development using chromatographic and mass spectral techniques for the analysis of small and macro molecules.
- Become skilled at de-convoluting and interpreting mass spectra of peptide/protein, including de-novo sequencing by MS/MS, calculation of
molecular weight from multiple-charge ion electrospray spectra, and other leading edge applications.

- Become familiar with data manipulation and data base searches through internet resources for the identification of unknown peptides and proteins.

**Course Topics**

- **Mass Spectrometry Fundamentals:**
  - mass, charge, creation of ions, mass spectrum, isotopes, fragmentation mechanisms and interpretation.

- **Ionization and sample introduction techniques:**
  - electron ionization (EI), Chemical ionization (CI), electro spray ionization (ESI), fast atom bombardment (FAB), matrix assisted laser desorption ionization (MALDI) techniques, HPLC, IC, GC etc.

- **Mass Spectrometric Analyzers:**
  - quadrupole, quadrupole ion trap; time-of-flight, detectors and vacuum systems.

- **Bio analytical methods based on modern MS:**
  - molecular weight determination, de novo sequencing of peptide/protein, peptide mass fingerprint (PMF), MS Tag, MS/MS, investigation of non-covalent interactions.
  - MALDI matrix considerations, effects of electrospray solvent systems, sample preparation procedures.

- **Protein database search and identification:**
  - Internet search engines, databases.