Advanced Mass Spectrometry CHM 5138 (3) [Core Analytical Course] Department of Chemistry & Biochemistry Florida International University

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Class Meets: Tuesday and Thursday 8:00 to 9:15AM GL272

Textbook: "Mass spectrometry: principles and applications" 3rd Edition. Edmond de Hoffmann and Vincent Stroobant.

Paperback edition: ISBN 978-0-470-03310-1, QD96.M3 H6413, 2007

Course Description: The class offers a in depth description of the processes and techniques involved in creating, controlling and measuring elemental or molecular ionic species by mass spectrometry techniques. Topics covered in the course include: Theory of mass spectrometry. Methods of ionization. Instrument Design. Combined Chromatography and Mass Spectrometry. Quantitative aspects of mass spectrometry. Meta-stable ions in mass spectrometry. Recent applications of mass spectrometry techniques (may involve some hands in experiments).

Learning outcomes: Students will become proficient with common concepts in mass spectrometry; understand the processes of ion formation, ion separation and detection. Students will obtain in-depth understanding of theory behind the principles of operation of mass analyzers and the conceptual design of common hyphenated mass spectrometry systems. Students will also be able to describe the fundamentals of both high resolution and multidimensional mass spectrometry.

Tentative Class outline:

Introduction to Mass Spectrometry (2 classes)

- · The mass spectrum
- Formation of ions
- Multipe Charged Species
- Isotopes
- · Metastable lons
- · Elemental composition of lons
- · Apperance of the mass spectrum

Theory of Mass Spectrometry (3 classes)

- · Energy States and Ionization
- · Formation of lons
- Theories of fragmentation rates
- · lons lifetimes
- · Qualitative Theories

Methods of ionization (4-5 classes)

- · Gas-Phase Ionization
- · Electron Ionization (EI)
- · Chemical Ionization (CI)
- · Desorption Chemical Ionization (DCI)
- · Negative-ion chemical ionization
- · Field Desorption and Ionization
- Field Desorption (FD)
- · Field Ionization (FI)
- · Particle Bombardment
- · Fast Atom Bombardment (FAB)
- Secondary Ion Mass Spectrometry (SIMS)
- Atmospheric Pressure Ionization
- · Electrospray Ionization (ESI)
- Atmospheric Pressure Chemical Ionization (APCI)
- · Laser Desorption
- · Matrix-Assisted Laser Desorption Ionization (MALDI)

Instrumental Design (2-3 classes)

- · Inlet systems
- · Ion sources
- · Mass analyzers basics (ion separators)
- · Detection and recording of spectra
- · Complete systems

Combined chromatography and mass spectrometry (3 classes)

- · Gas Chromatography/mass spectrometry (GC/MS)
- · Liquid chromatography/mass spectrometry (LC/MS)
- · Capillary electrophoresis/mass spectrometry (CE/MS)
- · Supercritical fluid chromatography/mass spectrometry (SFC/MS)
- Thin-layer chromatography/mass spectrometry (TLC/MS)
- · Other applications of mass spectrometry

Quantitative Mass Spectrometry (2 classes)

- · Introduction and principles
- · Specificity
- · Sensitivity and limits of detection
- · Calibration and standards
- Selected ion monitoring (SIM)
- · Selected reaction monitoring (SRM)
- Isotope dilution
- High-resolution vs. low-resolution
- · Accurate mass measurements
- · Derivatization

Non traditional Mass analyzers and tandem mass spectrometry (4-5 classes)

- · Unimolecular ion dissociation: Metastable ions
- · Collision-induced Dissociation (CID)
- · Double focusing magnetic sector instruments
- Triple Quadrupole instruments
- Three- and Four-sector instruments
- · Hybrid instruments
- Time of flight instruments
- · Ion traps
- · Fourier transform instruments
- · Tandem MS (MS^n)
- · Applications of MSⁿ

Student presentations – (2-3 classes)

Suggested reading material:

Journals

Analytical Chemistry Organic Mass Spectrometry International Journal of Mass Spectrometry and Ion Processes Biological Mass Spectrometry Mass Spectrometry Reviews Rapid Communications in Mass Spectrometry Journal of the American Society for Mass Spectrometry

Class assignment(s):

Students will be assigned a developmental mass spectrometry article to present and lead a class discussion. The presentation will be limited to 5 minutes and followed by 5 minutes for discussion. Student is required to provide, by e-mail, up to 2 power point slides the day before the presentation is due.

Final presentation/term paper:

Students will be required to make a 10-minute formal presentation or provide a term paper on a current emerging topic on mass spectrometry published in the literature in the last two years. All presentations must be made in Microsoft power point. A presentation schedule will be provided after the first mid-term exam.

Grading:

Midterm Exam	35%	October 11, 2011
Final Exam	35%	December 8 th 2011 7:30AM GL272
Paper/Presentation*	25%	
Assignment(s)	5%	

*Depending on the number of students in the class a term paper/presentation will be required.