CHEMISTRY 5138 Adv. Mass spectrometry

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Goal: to survey the theory and applications of mass spectrometry instrumentation

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).

Course Time MW 625-740
GC271A
Office Hours TTh 10-12

Text:
Additional materials
Various Handouts – distributed throughout the semester
Student lectures and presentations

Grades
1 Midterm 25%
1-2 Oral reports and a term paper 25%
Homework 20%
Final 30% comprehensive
Tests will cover book, lectures and readings from handouts.

Outline: Note: All topics are subject to change

	Monday	Wednesday
Week 1 August 24	Intro	Ion formation and elemental patterns – Chapter 6
Week 2 August 31	Intro to MS interpretation – Chapter 7	Theory 2 Basic interpretation -Chapter 7
Week 3 Sept 7	No class Labor day	Advanced Interpretation -Worksheet
Week 4 Sept 14	Ionization methods I - EI & CI Chapter 1	Ionization methods Electrospray and APCI - Chapter 1
Week 5 Sept 21	Ionization 3 Sims/laser desorption/ inorganic Chapter 1	No class
Week 6 Sept 28	Mass analyzers- Magnetic sectors and quadrupoles – Chapter 2	Student lectures 1
Week 7 Oct 5	Mass analyzers Ion traps, time of flight Chapter 2	Tandem MS/hybrid instruments Chapter 2/4
Week 8 Oct 12	Tandem MS applications Chapter 2/4	Exam I
Week 9 Oct 19	High resolution mass spectrometry Chapter 6	Student lectures 2
Week 10 Oct 26	Coupled systems GC/MS Chapter 5	HPLC/MS and CE/MS Chapter 5
Week 11 Nov 2	MALDi-TOF Chapter 1/5 Handouts	ICP/MS Chapter 1 and handouts
Week 12 Nov 9	Isotope ratio mass spectrometry Handouts	**Thursday Student lecture makeup day** Wed-no class – Veterans Day
Week 13 Nov 16	Student lectures 3	Quantitative mass spectrometry/analytical issues (chapter 6)
Week 14 Nov 23	Analysis of Biomolecules	Student lectures 4
Week 15 Nov 30	Biomolecules/ proteomics Guest lecturer	Review/ Student lectures 5
Week 16 Dec7	Finals	

Term papers, HW and Reports Due 1 week after your presentation. Score drops 1 letter grade for each week late.

Each student must prepare a 25 min overview on PowerPoint regarding a particular mass spectrometric topic or research paper. A 10-12 page review paper is also required.

The rules for the paper and presentations are as follows

1) Papers will be judged based on originality, insight and understanding of the topic, coherence of theme, grammar, and references.

2) Papers and presentations must be properly referenced according to the ACS style guide. For reference format see any ACS journal. Papers should be organized with an outline and should include a historical and scientific background, an overview of the topic, current applications of the topic, a critical review of the topic, conclusions and references.

3) References should be indicated by a number in brackets. References may consist only of books and scholarly articles. Important point!! References based on web sites may only be used if they reprint a scholarly article!!

4) Figures should be clear, properly labeled and referenced. Figure labels must stand alone and not require text to understand them. Figures must be referenced if not original.

5) For PowerPoint, there should be no more than 4 topics or lines of text on each slide, and all text should be clearly visible from the back of the room. This includes figure captions.

6) Scanned figures should be clear and legible – usually this means scanning in gray scale at 300 dots per inch. Should your pictures take up excessive memory, convert the figures to JPEG in Microsoft Photo editor and use the "more" feature in Microsoft photo editor to reduce the size of the figure. If labels on figures are too small, use the text editing features of powerpoint to write over them.

7) An electronic version of the paper and the powerpoint presentation must be submitted as well as a hard copy of the paper. These will be distributed to class members for further study. Again, the hardcopy paper is due one week after the presentation.

8) Plagiarism and/or use of research or reports from a previous class will result in a failing grade for the course. You may not report on topics involved in your current research project.

Suggested Topics (must involve publications in the past 3 -4 years)

Lecture set 1 theory and ionization

What is the theoretical basic of chemical ionization mass spectrometry?

Explain the theoretical basis of ion trap mass spectrometry

Explain the application of different chemical ionization methods for selective detection of biologically active compounds

Explain the role of nanospray MS in biomarker assays

Discuss the application of SIMS in the profiling of biological specimens

Explain the role of SIMS in the electronics and Materials industry

Lecture set 2 mass analyzers and MS designs

Discuss the application of glow discharge mass spectrometry for the analysis of solids

Contrast the application of electrospray ionization and atomospheric pressure ionization mass spectrometry in pharmaceutical analysis

Describe the current state of the art in portable mass spectrometry

Describe the development of ion trap and other MS devices for use in the Mars landers

Discuss the formation of heteronuclear cluster ions in atomic mass spectrometry

Discuss applications of ultrahigh resolution mass spectrometry.

Lecture set 3 tandem and coupled mass spectrometry

Discuss environmental applications of membrane introduction mass spectrometry

Discuss the development of DESI and DART techniques for screening chemical agents.

Explain the advantages of ion mobility time of flight mass spectrometry

Discuss the interfacing of microfluidic devices with mass spectrometry

Discuss TLC and maldi-TOF mass spectrometry

Explain the applications of orbitrap mass spectrometry

Describe QTOF and other hybrid mass spectrometry

Lecture set 4 MS applications

Describe the application of high resolution mass spectrometry in the petroleum industry.

Describe how metal ion speciation can be performed with HPLC/ICP/mass spectrometry

Discuss applications of Electrospray mass spectrometry in pharmaceutical QA/QC analysis

Describe the use of GC/MS in the determination of volatile aromatic hydrocarbons and in the detection of indoor air pollution

Describe applications of isotope ratio mass spectrometry in metabolic studies

Describe applications of isotope ratio mass spectrometry in oil exploration.

Lecture set 5 MS of biomolecules

Describe the application of MALDI-TOF in the determination of unknown bacterial spores?

Explain the application of Isotope ratio mass spectrometry in plant metabolism

Explain how the development of 2 dimensional mass spectrometry has revolutionized proteomics

Explain the effect of different matrices in the analysis of proteins by MALDI-TOF mass spectrometry

Discuss the development of electrospray mass spectrometry for the analysis of single nucleotide polymorphisms

How is mass spectrometry used to analyze whole cells

Explain the effect of ion adducts in electrospray mass spectrometry of peptides

Discuss recent applications of MALDI- TOF/TOF in denovo protein sequencing

Give a historical account of the development of mass spectrometry systems for proteomics.