

CHEM 6281/4803: Mass Spectrometry

Professor: Facundo M. Fernandez (facundo.fernandez@chemistry.gatech.edu, Office: ES&T Ford Building room L1-244 (lower level one).

Lectures: MWF 11:05 am - 11:55 am. Environmental Science and Technology (ES&T) L1-105 (lower level one).

Textbook: “Introduction to Mass Spectrometry. Instrumentation, Applications and strategies for Data Interpretation” by J. Throck Watson and O. David Sparkman. Fourth edition (2007), ISBN=978-0470516348, John Wiley and Sons.

Requirements: All the students enrolled in CHEM 6281/4803 are expected to conform to the Honor Code.

Course Description/Learning Objectives:

Students attending this course will obtain a complete understanding of the inner functioning of a modern mass spectrometer, and of modern MS techniques. We will explore the functioning of different mass analyzers, complemented by live ion-trajectory simulations. We will also focus on studying ion detectors and data acquisition systems. Special emphasis will be placed on the understanding of different tandem MS scan modes and their application in proteomics, forensics and drug discovery. Modern ionization methods such as MALDI and ESI will then be explained.

Grading system:

Students will be given one midterm and one final exam. Each exam will be graded in a 100-point scale and will account for 1/2 of the grade.

The final grade will be converted to a letter grade, based on the mean point grade, according to the following scale:

A (100 – 81 points); B (80 – 61 points); C (60 – 40 points); D (39 – 21 points); F (below 20 points).

Tentative Lecture Timeline:

Week	Tuesday
Week 1	Syllabus discussion. Intro to MS. Terminology. Example Applications (Chapter 1). Basic strategies for spectral interpretation (pg. 267-302). <u>No Class Aug 17 and 19 (ACS)</u>
Week 2	Basic strategies for spectral interpretation (cont'd). Isotopes
Week 3	TOF Mass Analyzers. TOF data acquisition. Hadamard TOF. (pg 53-82) <u>SIMION TOF simulations. No Class September 4th (CCE retreat)</u>
Week 4	3D and Linear Quadrupole Ion Trap Mass Analyzers. (pg 82-100) <u>SIMION QIT simulations. No Class Sept 7th (Labor Day)</u>
Week 5	Orbitraps and Transmission Quadrupoles. (pg 103-115) Ion Guides. <u>SIMION Q simulations.</u>
Week 6	FTICR analyzers (pg 122-127). Ion Detectors. Vacuum Systems(pg 136-162).
Week 7	<u>Catch up/Review week. No class Sept 28th-30th (Sci-X meeting)</u>
Week 8	Ion Mobility Spectrometry, theory, instrumentation and applications (pg 128-135). <u>No Class Oct 9th</u>
Week 9	October 12th: Review, Q&A. October 14th: Review, Q&A October 16th: Midterm.
Week 10	Electrospray Ionization. Chemical Ionization. DESI/DART (Chapter 7-8).
Week 11	MALDI. Instrumentation and Applications. MALDI Imaging (pg. 519-553).
Week 12	<i>Experiments in Fernandez Lab.</i> <u>No lecture.</u> October 26: Group 1 QiT. Group 2 TOF. Group 3: DART October 28: Group 1 DART. Group 2 QiT. Group 3: TOF October 30: Group 1 TOF. Group 2 DART. Group 3: QiT
Week 13	Ion activation techniques. Instrumentation for MS/MS. (pg. 173-192).
Week 14	Intro to spectral interpretation. Liquid Chromatography-Mass Spectrometry. (pg 639-676). Identification of unknowns based on accurate mass measurements.
Week 15	Spectral Interpretation (pg. 302-342).
Week 16	Intro to Proteomics (Chapter 12). <u>No Class Nov 25 and 27 (Thanksgiving)</u>
Week 17	Catch up
Finals week	Final Exam on Dec 9th (Wed) 8:00am - 10:50am
Week 19	Grades posted