

Faculty of Science Course Syllabus
Department of Chemistry
Chem 4206: Analytical Mass Spectrometry
Fall, 2018

Instructor: Dr. Alan Doucette alan.doucette@dal.ca Office: Chem 509

Lectures: MWF 9:35-10:25 Chem 223

Laboratories: None

Tutorials: None

Office Hours: By appointment

Course Description

This course offers a thorough treatment of modern analytical mass spectrometry instrumentation, with applications towards chemical and biochemical analysis. Specific examples include characterization of pharmaceuticals and biomolecules (proteins, carbohydrates), and discussion of field portable instruments. Reaction mechanisms and spectral interpretation are discussed, but are not emphasized in this applied course.

Course Prerequisites

CHEM 2201.03 (grade of C- or better)

Course Materials

- Recommended textbook: *Mass Spectrometry - A Textbook* by Jurgen H Gross, published by Springer Berlin Heidelberg. A free version of the entire textbook is available for download (link in course website)
- Course website: Brightspace. Included is a complete set of lecture notes, prerecorded lecture videos and other reference materials.

Course Assessment

The following grading scheme will be used for Chem 4206:

Component	Weight (% of final grade)	Date
<i>Test 1</i>	15%	<i>Oct 3 (50 min, in class)</i>
<i>Test 2</i>	15%	<i>Nov 5 (50 min, in class)</i>
<i>In class Presentation</i>	20%	<i>scheduled in November</i>
<i>Written Report</i>	15%	<i>Dec 4 (in class)</i>
<i>Final exam</i>	35%	<i>(Scheduled by Registrar)</i>

Other course requirements

Students should make every effort to attend all lectures and participate in discussions. Students will be required to meet with the instructor to discuss early drafts of their in-class presentation and report.

Conversion of numerical grades to Final Letter Grades follows the Dalhousie Common Grade Scale

A+ (90-100)	B+ (77-79)	C+ (65-69)	D	(50-54)
A (85-89)	B (73-76)	C (60-64)	F	(<50)
A- (80-84)	B- (70-72)	C- (55-59)		

Course Objectives/Learning Outcomes

- Use an exact MS or tandem MS spectrum to determine the formula of a molecule
- Discuss the concept of measurement uncertainty in an MS measurement
- Predict how resolution will influence the appearance of a mass spectrum
- List, identify and illustrate different types of ion sources and mass analyzers
- Appreciate the advantages/ disadvantages of different ion detectors when applied to MS
- Describe how and why molecules can be made to fragment by MS and how these fragments are detected.
- Explain how matrix effects influence detection sensitivity and how to overcome this.
- Infer how internal and external calibrants, and various sample preparation methods can improve the reliability of quantitative MS measurement
- Explain the physical principles that allow various types of mass analyzers to separate compounds by mass to charge.
- Discuss the advantages and limitations of various mass analyzers
- Explain the physical principles involved in the ionization of a molecule or atom, and how these principles can be used to create different ionization sources.
- Apply knowledge of the advantages/ limitations of various types of mass spectrometers to evaluate the merits of different MS instruments for different applications.
- Describe the chemical structure of a protein, and how it is related to function.
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- Understand how changes in a proteome impact the physiology of an organism.
- Contrast the difference between peptide fingerprinting and peptide mass mapping.
- Infer the importance of coupling separations to mass spectrometry.
- Rationalize the challenges in miniaturizing MS instrumentation.
- Perform literature-based research on a modern topic in mass spectrometry.
- Organize relevant information into a logical and informative presentation
- Generate a powerpoint presentation that illustrates and outlines a modern application of mass spectrometry
- Group information from independent research in the form of a written presentation.
- Critique student presentations
- Derive questions based on information presented in class

Course Content**INTRODUCTORY CONCEPTS (~5 lectures)**

- (a) Historical perspectives
- (b) The mass spectrum
- (c) Isotopes and isotope ratio calculations
- (d) Mass accuracy and resolution

QUANTITATIVE MASS SPECTROMETRY (~4 lectures)

- (a) Detectors and instrument noise
- (b) Tandem MS
- (b) Mass chromatograms
- (c) Quantitative measurements
- (d) Suppression and interferences

MASS ANALYZERS (~7 lectures)

- (a) Sectors/ TOF's
- (b) Quads/ Triple Quads/ qTOF's
- (c) Quadrupolar ion traps/ FTICR/ linear traps
- (d) The Orbitrap
- (e) Ion Mobility

IONIZATION TECHNIQUES (~5 lectures)

- (a) EI/ CI
- (b) Desorption/ MALDI
- (c) Electrospray

APPLICATIONS (~6 lectures)

- (a) Small molecule/ fragmentation
- (b) Proteomics
- (c) Environmental monitoring/ Field portable instruments

STUDENT PRESENTATIONS (~5 lectures)

List of potential topics is provided.
Topics explore modern applications of mass spectrometry.
First student presentation tentatively scheduled for March 18.

NOTE: You are also responsible for the material delivered through the student presentations. This will be covered on your final exam.

Course Policies

If, due to illness, the student will miss a scheduled appointment, a presentation, or in-class test, he/she must contact the instructor prior to the missed appointment. The presentation/ appointment will be rescheduled at the next available opportunity. Arrangements *may* be made to accommodate a makeup test. The instructor reserves the right to prorate the remaining assessment components to determine a final grade. Please note that the makeup test may not necessarily be identical to the original test, and may be conducted in the form of an oral examination, at the discretion of the instructor.

If the student misses the final exam, the instructor must be notified within 24 hours, at which point a makeup will be scheduled at the earliest possible time. A student declaration of absence form must be handed to the instructor in the case of illness affecting any graded assessment component.

Students will be returned all written forms of assessment (tests, assignments), following grading within 7 days of their submission. The final exam will not be returned to the students, though students are welcome to view their graded exam through appointment with the instructor.

The instructor will communicate any relevant course information through the course website. Please check this site regularly for announcements and new content.

ACCOMMODATION POLICY FOR STUDENTS

Students may request accommodation as a result of barriers related to disability, religious obligation, or any characteristic protected under Canadian Human Rights legislation. The full text of Dalhousie's Student Accommodation Policy can be accessed here:

http://www.dal.ca/dept/university_secretariat/policies/academic/student-accommodation-policy-wef-sep--1--2014.html

Students who require accommodation for classroom participation or the writing of tests and exams should make their request to the **Advising and Access Services Centre (AASC)** prior to or at the outset of the regular academic year. More information and the ***Request for Accommodation*** form are available at www.dal.ca/access.

ACADEMIC INTEGRITY

Academic integrity, with its embodied values, is seen as a foundation of Dalhousie University. It is the responsibility of all students to be familiar with behaviours and practices associated with academic integrity. Instructors are required to forward any suspected cases of plagiarism or other forms of academic cheating to the Academic Integrity Officer for their Faculty.

The Academic Integrity website (<http://academicintegrity.dal.ca>) provides students and faculty with information on plagiarism and other forms of academic dishonesty, and has resources to help students succeed honestly. The full text of Dalhousie's ***Policy on Intellectual Honesty*** and ***Faculty Discipline Procedures*** is available here:

http://www.dal.ca/dept/university_secretariat/academic-integrity/academic-policies.html

STUDENT CODE OF CONDUCT

Dalhousie University has a student code of conduct, and it is expected that students will adhere to the code during their participation in lectures and other activities associated with this course. In general:

“The University treats students as adults free to organize their own personal lives, behaviour and associations subject only to the law, and to University regulations that are necessary to protect

- the integrity and proper functioning of the academic and non – academic programs and activities of the University or its faculties, schools or departments;
- the peaceful and safe enjoyment of University facilities by other members of the University and the public;
- the freedom of members of the University to participate reasonably in the programs of the University and in activities on the University's premises;
- the property of the University or its members.”

The full text of the code can be found here:

http://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

SERVICES AVAILABLE TO STUDENTS

The following campus services are available to help students develop skills in library research, scientific writing, and effective study habits. The services are available to all Dalhousie students and, unless noted otherwise, are free.

Service	Support Provided	Location	Contact
General Academic Advising	Help with <ul style="list-style-type: none"> - understanding degree requirements and academic regulations - choosing your major - achieving your educational or career goals - dealing with academic or other difficulties 	Killam Library Ground floor Rm G28 Bissett Centre for Academic Success	In person: Killam Library Rm G28 By appointment: <ul style="list-style-type: none"> - e-mail: advising@dal.ca - Phone: (902) 494-3077 - Book online through MyDal
Dalhousie Libraries	Help to find books and articles for assignments Help with citing sources in the text of your paper and preparation of bibliography	Killam Library Ground floor Librarian offices	In person: Service Point (Ground floor) By appointment: Identify your subject librarian (URL below) and contact by email or phone to arrange a time: http://dal.beta.libguides.com/sb.php?subject_id=34328
Studying for Success (SFS)	Help to develop essential study skills through small group workshops or one-on-one coaching sessions Match to a tutor for help in course-specific content (for a reasonable fee)	Killam Library 3rd floor Coordinator Rm 3104 Study Coaches Rm 3103	To make an appointment: <ul style="list-style-type: none"> - Visit main office (Killam Library main floor, Rm G28) - Call (902) 494-3077 - email Coordinator at: sfs@dal.ca or - Simply drop in to see us during posted office hours All information can be found on our website: www.dal.ca/sfs
Writing Centre	Meet with coach/tutor to discuss writing assignments (e.g., lab report, research paper, thesis, poster) <ul style="list-style-type: none"> - Learn to integrate source material into your own work appropriately - Learn about disciplinary writing from a peer or staff member in your field 	Killam Library Ground floor Learning Commons & Rm G25	To make an appointment: <ul style="list-style-type: none"> - Visit the Centre (Rm G25) and book an appointment - Call (902) 494-1963 - email writingcentre@dal.ca - Book online through MyDal We are open six days a week See our website: writingcentre.dal.ca