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Faculty of Science Course Syllabus
Department of Chemistry
Chem 4206: Analytical Mass Spectrometry
Fall, 2022

Dalhousie University is located in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq. We are all Treaty people.

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

Office Hours: I have no set office hours, but you are always welcome to drop by office, or to email me to schedule an appointment at your convenience.

Lectures: MWF, 12:35 pm – 1:25 pm (AST). ROOM: LSC-OCEANOGRAPH O3655
All lectures are live-streamed and recorded through the Teams course site.
Also available are pre-recorded videos on my YouTube Channel (ShortChemistry)

Laboratories: None

Tutorials: Additional help sessions will be offered as needed ahead of midterms and final exam

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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)

Cross listing

Chem 5206.03

Course Materials

- Course website: Brightspace. Included is a complete set of lecture notes, pre-recorded lecture videos, problem sets and other reference materials.
- There are several excellent textbooks on mass spectrometry for those looking to supplement their reading. I would recommend any of the following:
  (1) Mass Spectrometry - A Textbook by Jurgen H Gross, published by Springer.
  (2) Mass Spectrometry – Principles and Applications by Edmond de Hoffmann and Vincent Stroobant, (John Wiley & Sons).
  (3) Mass Spectrometry: A Foundation Course by Kevin Downard (Royal Society of Chemistry).

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(course materials continued)

Some of the above texts 'may' be available online as free downloadable pdf files. While copyright laws prevent me from posting a direct link, those who are willing to search may find a copy. I personally own all three of these books. They can also be purchased from independent sites such as Amazon, or directly from the publisher.

Communication

Announcements related to the course will be communicated through the course website. Additionally, please use and check your Dalhousie email for course related communications.

Course Assessment

The following grading scheme will be used for Chem 4206:

Component	Weight (% of final grade)	Date
Midterm 1	*15 or 20 % [(a)]*	*Oct 12 (12:30 – 1:30 pm) [(b)]*
Midterm 2	*15 or 20 % [(a)]*	*Nov 21 (12:30 – 1:30 pm) [(b)]*
Presentation	*20%*	*Last ~ 3 weeks of lectures*
Written Report	*10%*	*Dec 7 (5 pm)*
Final exam	*35%*	*(Scheduled by Registrar) [(c)]*

[(a)] *The highest of your two tests will be weighted 20%, and the lowest 15%.*

[(b)] *Makeup test date tentatively scheduled for the day following original test.*

[(c)] *All testing will be conducted in person. You will not have access to your notes, but you will be provided appropriate data tables, equations, and online calculators when necessary.*

Other course requirements

All students will be required to meet with the instructor (in person, or on Teams) as part of a small group (~1 hour) as part of the preparation for their in-class presentation.

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)	

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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.
- 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

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Course Content

Week 1: Sept 7-9
Course expectations; MS basics; Historical overview of mass spectrometry

Week 2: Sept 12-16
The mass spectrum; Isotopes; Isotope ratios; Mass resolution

Week 3: Sept 19-23
Exact mass calculations; Formula determination; MS detectors

Week 4: Sept 26-Sept 28
Quantitative analysis; Coupling MS to separations; Mass chromatograms

Week 5: Oct 3-7
Mass analyzers I: Sectors; Time of flight, Quadrupoles

Week 6: Oct 12-14 (Midterm 1)
Mass analyzers II: Quadrupoles

Week 7: Oct 17-21
Mass analyzers III: Ion cyclotron resonance; Orbitrap; hybrid instruments (eg Q TOF);

Week 8: Oct 24-28
Ionization modes: Electron vs Chemical ionization, MALDI, Electrospray, Passive sampling

Week 9: Oct 31- Nov 4
Application I: Ion Mobility Spectrometers; Small molecule fragmentation

Week 10: Nov 7-11 **STUDY BREAK**

Week 11: Nov 14-18
Application II: Proteomics

Week 12: Nov 21-25 (Midterm 2)
Student Presentations I

Week 13: Nov 28-Dec 2
Student Presentations II

Week 14: Dec 5 – 7
Student Presentations III

NOTE: *You are responsible for the material delivered in the student presentations (tested on final exam).*

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University Policies and Statements

This course is governed by the academic rules and regulations set forth in the University Calendar and by Senate

Missed or Late Academic Requirements due to Student Absence

If, due to illness, the student will miss a scheduled meeting, presentation, test or final, the student must contact the instructor **prior to** the missed appointment. The presentation will be rescheduled to the next available opportunity. If the makeup test is also missed, marks will be redistributed to other assessment components to determine a final grade. Please note that the makeup test may not necessarily be identical to the original test.

If the student misses the final exam, the instructor must be notified within 24 hours, at which point a makeup will be scheduled at a mutually agreeable time.

As per Senate decision instructors may not require medical notes of students who must miss an academic requirement**, including the final exam**, for courses offered during fall or winter 2020-21 (until April 30, 2021). A student declaration of absence form must be handed to the instructor in the case of illness affecting any graded assessment component. Information on regular policy, including the use of the Student Declaration of Absence can be found here: **https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.html.**

Academic Integrity

At Dalhousie University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity.
Information: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Advising and Access Services Centre is Dalhousie's centre of expertise for student accessibility and accommodation. The advising team works with students who request accommodation as a result of a disability, religious obligation, or any barrier related to any other characteristic protected under Human Rights legislation (Canada and Nova Scotia).
Information: https://www.dal.ca/campus_life/academic-support/accessibility.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner—perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution.
Code: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness
Statement: http://www.dal.ca/cultureofrespect.html

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Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel and support. Visit or e-mail the Indigenous Student Centre (1321 Edward St) (elders@dal.ca).
Information: https://www.dal.ca/campus_life/communities/indigenous.html

Important Dates in the Academic Year (including add/drop dates)
https://www.dal.ca/academics/important_dates.html

University Grading Practices
https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html

Student Resources and Support

Advising

General Advising https://www.dal.ca/campus_life/academic-support/advising.html

Science Program Advisors: https://www.dal.ca/faculty/science/current-students/academic-advising.html

Indigenous Student Centre: https://www.dal.ca/campus_life/communities/indigenous.html

Black Students Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html

International Centre: https://www.dal.ca/campus_life/international-centre/current-students.html

Academic supports

Library: https://libraries.dal.ca/

Writing Centre: https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html

Studying for Success: https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html

Copyright Office: https://libraries.dal.ca/services/copyright-office.html

Fair Dealing Guidelines https://libraries.dal.ca/services/copyright-office/fair-dealing.html

Other supports and services

Student Health & Wellness Centre: https://www.dal.ca/campus_life/health-and-wellness/services-support/student-health-and-wellness.html

Student Advocacy: https://dsu.ca/dsas

Ombudsperson: https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html

Safety

Biosafety: https://www.dal.ca/dept/safety/programs-services/biosafety.html

Chemical Safety: https://www.dal.ca/dept/safety/programs-services/chemical-safety.html

Radiation Safety: https://www.dal.ca/dept/safety/programs-services/radiation-safety.html

Scent-Free Program: https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html

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A Presentation on Current Topics in Mass Spectrometry (Fall, 2022)

Your presentation is intended to outline a *current topic* in the field of mass spectrometry. The suggested topics are meant to complement, but not duplicate the material already covered in this class (see course outline). You will be presenting your topic individually and are given the choice of giving a live presentation (in class), or creating a pre-recorded video, such as those I have posted on YouTube. Regardless of the method of delivery, other students from the Chem 4206/ 5206 students will watch your presentation and together with the instructor, will ask questions at the conclusion of your presentation.

All students enrolled in Chem 4206/5206 are responsible for the material you will personally present through your lecture. This material will be examined on the final exam. No two presentations will cover the same material. As your presentation is an integral component of this class, it as my objective to ensure that every student does the best job possible, not only in the delivery of the material, but also in determining the specific content to emphasize. In addition to your presentation, your slides/ recording will be made available to the class as part of their collection of course reference material.

Presentation Format:

All presentations and associated discussions will take place after the second midterm, occupying the bulk of lecture time (Nov 23 – Dec 7). Your final presentation date will be selected by the instructor. Each presentation should aim to be 15-20 min long, allowing ~10 min of question & discussion from the audience (including the instructor). Live presentations must be conducted using Powerpoint or similar electronic format (no 'chalk talks'). Pre-recorded videos may involve a multitude of visual aids. Your presentation file (slides, video) should be uploaded to the instructor a minimum 24 hours prior to your presentation, which will be shared with the class. Pre-recorded videos will only be posted to YouTube upon written permission by the student.

Workshops:

To aid the development of your presentation, you will work with the instructor and members of the class. Your first task is to pick a topic and will involve a short meeting with the instructor. This can be done via email exchange, but ideally should involve a discussion with the instructor. You should have selected one or two key references and outline the general topic you wish to cover. Remember no two topics can be identical. Topics must be approved by the instructor, and occur on a first come, first serve basis.

You will next participate in a presentation workshop, (scheduled during class time Oct 28. This workshop is intended to share a 'rough outline' of your presentation, seeking feedback from a group of your peers. You should have a general sense of the material you want to discuss, with a few sample visuals (*eg* a couple of slides) to demonstrate the final look and style of your presentation. I will also meet with you (outside of class) to provide some early feedback.

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Workshops continued:

For those intending live presentations, your second workshop will be scheduled outside of class at a mutually agreed time (~1 hour, minimum 1 week prior to final talk). Together with a small group of your peers (typically 2-3 at a time), you will deliver a formal 'practice talk', with feedback from your peers and instructor. The aim of these meetings is to make final tweaks to your presentation and ensure that everyone does the best possible job in clearly presenting their material, while ensuring that relevant material is presented for the benefit of the class.

For those intending a pre-recorded video, the above-described workshop should take place prior to recording your video and will involve a 'dry run' of your talk, overlaid with your visual aids. It is recommended that this meeting takes place a minimum 2 weeks prior to your final presentation.

Summary of Dates:

Topic Selection: The earlier the better! Your final deadline for topic approval is Oct 7.

Workshop 1: Oct 28. In class (plus a 1-on-1 meeting with instructor outside of class).

Workshop 2: ~1 week prior to your class presentation, or 2 weeks prior to pre-recorded presentations. Meeting times to be scheduled with your group at mutually agreed times.

Assessment:

The presentation constitutes 20 % of your total grade, with breakdown as follows:

a) Workshop #1 (rough outline)	2 marks
b) Workshop #2 (full practice)	6 marks
c) Formal presentation	12 marks

A detailed grading sheet will be provided at a later date. Note that in the practice talk, presented during your second workshop, I will not emphasize your delivery of the material. Also, since pre-recorded talks have the opportunity for multiple takes and/or edit mistakes, the standards of your delivery will be higher than a live presentation. Components of your presentation that factor into the final grade include:

- *Depth and implications of science*
- *Interest level of the content presented*
- *Speaking style and enthusiasm*
- *Quality of visual aids*
- *Your level of understanding of the material (based on audience questions)*

Topic Selection:

A list of past topics is provided as a general guide, however you are free to pick any topic with an emphasis on mass spectrometry. A literature search (science citation index / web of science) of your topic would be a good place to start, as I am sure it will yield numerous hits. I do not mind if the topic is close to your own interests or research – in fact, I highly encourage it! But you should

not be presenting data generated directly from your personal research. If you're stuck on a topic, please meet with me to discuss.

Once you have selected a potential topic, you must meet with me to discuss the idea. All topics must be approved by the instructor. Include a minimum of two peer-reviewed references (please attach links to these references) and a descriptive title for your presentation. It would be helpful to also provide a short paragraph description of what you hope to cover. Topics will be assigned on a first come, first serve basis, with a tentative presentation date determined by the instructor. No two presentations will cover the identical material.

***** Deadline for *selection and approval* of your topic is Friday Oct 7 *****

Late topic selections will result in a 1-point daily deduction from your total presentation grade.

List of potential topics (for inspiration – your choice can be anything!)

1. Metabolomics / lipidomics or other 'omics fields
2. Canada's Contributions to Mass Spectrometry
3. Intact protein analysis (top-down proteomics)
4. New modes of MS ionization/ detection / fragmentation
5. Miniature Mass Spectrometers/ Field Portable Devices
6. MS in the military / Detection of chemical / biological weapons
7. Food Science – application or certification
8. MS for dating samples/ stable isotope ratios / accelerator MS
9. Protein Quantitation (relative or absolute methods)
10. High resolution mass spectrometry
11. Toxicology
12. MS Imaging
13. Protein conformational analysis – HD exchange
14. MS in pharmaceuticals
15. Fragmentation Mechanisms of organic compounds
16. Elemental analysis – ICP/MS
17. Bioinformatics/ MS data analysis
18. Newborn Screening
19. Historical Overview of Mass Spectrometry
20. Social impacts where mass spectrometry may contribute

I recommend you approach the topic by first ignoring mass spectrometry and thinking about what interests you. From there, see how mass spectrometry may be involved with that topic. You might be surprised how widespread this technology is today.

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Written Assignment (Chem 4206)

You will write a formal report, describing the same topic that was covered in your oral presentation. While the report covers essentially the same material, it should be recognized that written communication is a different medium than a highly visual presentation. Additionally, communication starts by recognizing your audience. While your presentation is intended to be delivered at a level suitable for an advanced scientific audience (ie your peers in this class), your written presentation is intended for a more general audience. Think someone who just completed their first year of a science degree at Dal. You have perhaps encountered scientific **blogs**. Here are some examples:

https://www.sciencealert.com/
http://blogs.nature.com/ http://www.chemistry-blog.com/tag/jacs/
https://blog.sepscience.com/massspectrometry
http://proteomicsnews.blogspot.com/
https://theconversation.com/ca

These short, web-based articles outline scientific discoveries (typically those originally presented in peer-reviewed articles) but for a more general audience (the original articles are not only long but can be quite complex to understand). They also tend to place stronger emphasis on the importance of the work for their intended audience. Such a form of science communication not only improves public awareness of this area of research but enhances science literacy, which better informs individuals as well as policy makers to arrive at appropriate decisions

You will prepare a science blog, with a strict limit of **1000 words**. The blog should contain a 'catchy' title (different than the title of the article) and reference the original work. The report should be prepared in Microsoft Word (single column, double spaced, 12 pt Times New Roman font). You may use subheadings where appropriate to break up the main topics of your report.

Your blog must include (at least) one original figure. This figure can incorporate components taken from other sources (including the article) and will aim to provide the reader with a quick overview of the work and its relevance (do not copy the article abstract image). Additional figures can be included within the article (max 2, not including main image), with short tag lines describing them.

The blog should emphasize the impact of the work. It should also provide a summary of the study's design and main findings. Make sure to give a brief explanation of how mass spectrometry was used in this work (at a general level). Do not feel you should avoid the use of proper scientific terminology – just don't make it too complicated.

I encourage you to share your blog with others from outside the class for their feedback. And while it is not essential for your report, I also encourage you to contact the original authors of your study. I will provide a list of possible questions that you can use to interview the

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authors (perhaps by email, or even on a Zoom call). You can include original quotes from the authors, with their permission.

Deadlines:
The blog is due on the last day of term (Dec 7, 5 pm). You can seek feedback from the instructor by providing an early draft of your blog up until Nov 28 (5 pm). While this draft is optional, you should look at it like this. I will provide you with my comments, to let you know exactly what you can do to improve your writing. There is no cost to you, other than insuring you submit a draft by the deadline.

Grading:
The following breakdown will be used to assess your blog. The report itself is worth 5% of your total grade in this course.

STYLE (25%)
Basic grammar, sentence structure, referencing, format

STRUCTURE (25%)
The overall 'flow' of document, paragraph structure, conveying a clear message, easy to read, with figures complementing the story

INTEREST (25%)
Did the blog clearly convey the relevance of the work to a non-science audience? Was the science presented in a way that the public would understand and appreciate it?

DEPTH (25%)
Includes sufficient depth of the experiment design, methodology, and principle findings, as they pertain to the topic of mass spectrometry.