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Faculty of Science Course Syllabus
Department of Chemistry
Chem 5206: Bioanalytical Mass Spectrometry
Fall, 2020

Instructor: Dr. Alan Doucette alan.doucette@dal.ca Office: my kitchen table

Office Hours: Monday, 11:30 – 12:30 pm & Thursday 9:00 – 10:00 am [1]

** Or make a request for a specific appointment. These are meant as administrative appointments and will be conducted through Microsoft Teams. For help related to class content, please refer to tutorial sessions.*

Lectures: Asynchronous videos (links available through Brightspace) + synchronous tutorials.

Beginning November 16th, this class will shift to synchronous lectures, MWF, 11:35 am – 12:25 pm. These times relate to student presentations, with details provided later in this syllabus.

Laboratories: None

Tutorials: Optional. Synchronous delivery via Microsoft Teams

2 x 1 hr tutorials are offered weekly: Wednesday & Friday, 11:30 am - 12:30 pm (until November Study Break). After this break, weekly tutorials will be scheduled at a time that best meets the availability of the class.

[1] *All times listed in this syllabus are in Atlantic Standard Time (AST)*

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) or instructor approval

Cross listing

Chem 4206.03

Course Materials

- Course website: Brightspace. Included is a complete set of lecture notes, pre-recorded lecture videos, problem sets and other reference materials.

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(Course Materials continued)

- There are several excellent textbooks on mass spectrometry for those looking to supplement their reading. I didn't request any through the bookstore as they are rather expensive and/or contain far more information than required for this course. However, I would recommend any of the following as a supplement to the course material or for reference:

  (1) *Mass Spectrometry - A Textbook* by Jurgen H Gross, published by Springer Berlin Heidelberg.
  (2) *Mass Spectrometry – Principles and Applications* by Edmond de Hoffmann and Vincent Stroobant, published by John Wiley & Sons, Chichester.
  (3) Mass Spectrometry: A Foundation Course by Kevin Downard (Royal Society of Chemistry).

  Some of the above texts have been found online as free downloadable pdf files. Unfortunately, copyright laws prevent me from posting a direct link, but to those willing to hunt, you will likely find them. The books 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	*10 or 15 % [(a)]*	*Oct 7 (11:30 – 12:30 pm) [(b)]*
Midterm 2	*10 or 15 % [(a)]*	*Nov 6 (11:30 – 12:30 pm) [(b)]*
Presentation	*20%*	*To be scheduled outside class time, (towards end of term)*
Written Report	*25%*	*Dec 8 (5 pm)*
Final exam	*30%*	*(Scheduled by Registrar) [(c)]*

[(a)] *The highest of your two tests will be weighted 15%, and the lowest 10%.*
[(b)] *Makeup test dates are Oct 8 & Nov 17 (4:00-5:00 pm)*
[(c)] *Final exam and midterms will be conducted remotely. Copies of the test will be provided as a downloadable file which can be completed electronically, or printed out and written by hand (upload photos when finished). Additional time will be provided to upload files once complete. All tests and final exam will be 'open book', and must be completed individually.*

Other course requirements

All students will be required to meet with the instructor (Microsoft Teams) on a minimum two separate occasions (~15 min per meeting) to discuss early drafts of their in-class presentation.

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

A+ (90-100)	**B+** (77-79)	
A (85-89)	**B** (73-76)	
A- (80-84)	**B-** (70-72)	F (<70)

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 8-11
Course expectations; MS basics; Historical overview of mass spectrometry

Week 2: Sept 14-18
The mass spectrum; Isotopes; Isotope ratios; Mass resolution

Week 3: Sept 21-25
Exact mass calculations; Formula determination; MS detectors

Week 4: Sept 28-Oct 2
Quantitative analysis; Coupling MS to separations; Mass chromatograms

Week 5: Oct 5-9 ***(Midterm 1)***
Mass analyzers I: Sectors; Time of flight; Quadrupoles

Week 6: Oct 12-16
Mass analyzers II: Ion cyclotron resonance; Orbitrap; hybrid instruments (eg Q TOF); Ion mobility

Week 7: Oct 19-23
Ionization modes: Electron vs Chemical ionization, MALDI, Electrospray, Passive sampling

Week 8: Oct 26-30
Application I: Small molecule fragmentation

Week 9: Nov 2-6 ***(Midterm 2)***
Application II: Proteomics

Week 10: Nov 9-13 **STUDY BREAK**

Week 11: Nov 16-20
Student Presentations I (Synchronous lectures)

Week 12: Nov 23-27
Student Presentations II (Synchronous lectures)

Week 13: Nov 30 – Dec 4
Student Presentations III (Synchronous lectures)

Week 14: Dec 7-8
Review of material for final exam

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, 2020)

Your presentation is intended to outline a *current topic* in the field of mass spectrometry. The suggested topics are meant to complement the material from the course outline. You will present your topic though synchronous presentations in Microsoft Teams. Other students from the Chem 4206/ 5206 students will be in attendance and will ask questions at the conclusion of your presentation.

All students enrolled in Chem 5206 are responsible for the material you will present through your lecture. This material will be examined on the final exam. Since this is the case, it is my objective to ensure every student does the best job possible, not only with the delivery of the material, but in determining the specific content to emphasize. In addition to your presentation, your slides will be made available to the class as part of their collection of course reference material.

Presentation Format:

With such a large class this year, it may not be possible to host your presentations in front of the full 4206/5206 class (during synchronous lecture time). I will likely need to organize separate meetings outside our regular class time, and invite all 5206 students to attend class. Your presentation must be between 40-45 minutes in length, to be followed by ~10 min of question and discussion from the audience (including the instructor). The presentation must be conducted through Powerpoint (or similar format – no 'chalk talks'). The presentation file should be emailed to the instructor at least 24 hours prior to your presentation, such that the slides can be posted to the course website.

Students are required to meet with the instructor on two separate occasions. The first meeting (~15 min) is intended to go over a 'rough outline' of your presentation. You should have a sense of the material you want to discuss on a slide-by-slide basis. I will provide suggestions to improve your presentation, and may ask that you cover additional material, or omit some. The second meeting (minimum 1 week prior to final presentation) will include a formal 'practice talk', including feedback from the instructor and at least 1 classmate. The aim of these meetings is to ensure that everyone does the best possible job with their talks, and to ensure that appropriate material is presented for the benefit of the class.

Dates for meeting 1 & 2:

1st meeting: minimum 3 weeks before your presentation (Microsoft Teams)
2nd meeting: minimum 1 week before your presentation, to be presented in front of a smaller class audience. A signup sheet of possible times for these meetings will be posted shortly.

Assessment:

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

a) 1st meeting to discuss topic/ review presentation	2 marks
b) 2nd meeting with full 'practice' talk	6 marks
c) Formal presentation	12 marks
Depth/ interest level of material	
Speaking style / slide quality	

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Level of understanding of material (based on audience questions)

Topic Selection:

A list of potential topics is provided, 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 research – in fact, I welcome it! But you should not be presenting data obtained through your "own" work. If you're stuck on a topic, please meet with me to discuss.

Once you have selected a potential topic, you must email me your topic for approval. This includes a minimum of 2 reference (attach copies of the full references) and a descriptive title. 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 2 *****

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

The above list is but a partial representation of the versatility of mass spectrometry. You are welcome to choose any topic you find interesting, including ones not on this list.

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Written Report (Chem 5206)

You are asked to write a mini scientific review of the same general topic that you will present in class. The review should therefore be a direct complement to your seminar. While the research that went into your topic might be the same, the format of a written review allows you to cover the material in a slightly different way. Your writing style should be formal, using properly formatted paragraphs (*ie* do not write in point form!). The material you describe must be fully cited, with references included at the end of the report, in proper scientific format. Websites may be used for some of your references, though you must include a minimum of eight peer-reviewed scientific publications amongst your reference list

Your report will have a strict limit of **4000 words** (not included reference). The report should be prepared in Microsoft Word (single column, double spaced, 12 pt Times New Roman font). Use subheadings as appropriate to break up the main topics of your report.

Your report must also include the following:

(1) **A descriptive title**: <120 characters
(2) **Abstract**: < 150 words, summarizing the most important aspects of your review
(3) **Keywords**: 5-10
(4) **Background**: Provide immediately relevant background on your chosen topic. Note that this is a focused mini review, and so you cannot cover everything in your background. The first paragraph should very quickly funnel down from the broader field to your specific topic. Get to the point as quickly as you can, so that you have more opportunity to expand on that specific area.
(5) **Main Body**: (include subheadings where appropriate). Your literature review is presented in this section. Focus on recent works (preferably in the last 5 years). Do not attempt to cover too many articles. I suggest no more than 10, but it could be as few as 3. Include relevant figures or tables (taken straight from your referenced articles) as appropriate. I expect a minimum of 2 figures or tables, but no more than 8 in total. Figure captions and table headers are included in your word count limit.
(6) **'Personal' Commentary and 5-year outlook:** This section should be brief (a paragraph or two), where you discuss the advantages and limitations of the topic, and where future research is heading.
(7) **Concluding Remarks**: This is not meant to be a summary of the review (that's what the abstract is for). Instead, this short section (~100-150 words) should provide some comments on what the reader should take away from this topic. Where does the future lie in this area? Is this an up-and-comer, or has the technique seen better days? What problems remain to be overcome? How does it compare/compete against other related methods?
(8) **References**: Reference formats are specific to journals. Being an analytical chemistry class, you should follow the format of the journal *Anal. Chem.* Use original articles, or books (website references may be ok if they are the primary source). I'm guessing 20-30 references.

Deadlines:

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The report is due on the last day of class (Dec 8, 5pm). Up to two draft copies of the written report can be submitted to the instructor for feedback. These drafts are not graded, but the feedback will surely help you in preparing the final report.

Deadline for submission of a 1st draft: Nov 2, 2020
Deadline for submission of a 2nd draft: Nov 23, 2020

Grading:
The following breakdown will be used to assess your report. The report itself is worth 25% of your total grade in this course.

STYLE (25%)
Basic format, referencing, figure/ table layout, font styles and grammar

STRUCTURE (25%)
The overall 'flow' of document, paragraph structure, conveying a clear message, easy to read…

DEPTH (50%)
Includes sufficient depth, with material relevant to the overall objectives of this class.