

Faculty of Science Course Syllabus  
Department of Chemistry  
Chem 5206: Bioanalytical 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](mailto:alan.doucette@dal.ca)      Office: CHEM 509

**Office Hours:** I have no set office hours, but you are always welcome to pop into my office, or just email me to schedule an appointment at your convenience.

**Lectures:** MWF, 12:35 pm – 1:25 pm (AST). ROOM: LSC-OCEANOGRAPH O3655

Lectures are also 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 are typically offered 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. Students directly shape the content of this class through the delivery of their individual in-class presentations.

### Course Prerequisites

CHEM 2201.03 (grade of C- or better)

**Cross listing:** Chem 4206.03

### Course Materials

- Course website: Brightspace (accompanied by my YouTube channel, ShortChemistry). Included is a complete set of lecture notes, pre-recorded lecture videos, problem sets and recommended reference materials.

- Several excellent textbooks on mass spectrometry are available for those looking to supplement their reading. While none will be available through the Dalhousie Bookstore, these books are available through our library.

- (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 <sup>(a)</sup>

Component	Weight (% of final grade)	Date
<i>Midterm 1</i>	15 % <sup>(b)</sup>	<i>Oct 12 (in class) <sup>(c)</sup></i>
<i>Midterm 2</i>	15 % <sup>(b)</sup>	<i>Nov 21 (in class) <sup>(c)</sup></i>
<i>Presentation</i>	25%	<i>To be scheduled during class time At end of term (Nov/ Dec)</i>
<i>Written Report</i>	20%	<i>Dec 16 (5 pm)</i>
<i>Final exam</i>	25% <sup>(b)</sup>	<i>(Scheduled by Registrar) <sup>(d)</sup></i>

<sup>(a)</sup> I will consider shifting relative weighting of your midterms + final, but they will add up to 55%

<sup>(b)</sup> You will write the identical midterms as 4206, but be given additional question(s) on the final.

### Other course requirements

All students will be required to meet with the instructor (in person or Microsoft Teams), approximately 1-2 weeks prior to their in-class presentation (max 1.5 hours) to provide and receive feedback on student presentations.

**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)

*\*\* Note your minimum  
pass grade is >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 and deliver a visual presentation that illustrates and outlines a modern application of mass spectrometry
- Conduct a thorough and critical review of a current topic in mass spectrometry, summarized in a formal written report taking the form of a peer-reviewed article.
- Critique student presentations
- Derive questions based on information presented in class

### **Missed or Late Academic Requirements due to Student Absence**

At this time, we remain in a pandemic, with several restrictions and recommendations described by Nova Scotia Public Health and by Dalhousie University. This includes policies on mask wearing, vaccination, testing, and physical distancing. All students are required to comply with health and safety requirements on campus and should be considerate of others' health concerns. Non-compliance may be reported under the Code of Student Conduct.

While the return to campus still brings some uncertainties, our expectations are that the campus will remain open. This does not preclude the fact that individuals may still be affected. As recommended by public health, if you are feeling ill or displaying flu-like symptoms, you should stay home. It is for this precise reason that all lectures will be available in person as well as remotely. You may also prefer to meet with me online rather than in person. This will also be accommodated.

If, due to illness, you are unable to attend a scheduled meeting, presentation, or midterm, you must contact the instructor **prior to** the missed event. A [student declaration of absence form](#) is required for any graded component. Makeup test dates are posted, while your 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 you miss the final exam, the instructor must be notified within 24 hours, and a student declaration of absence form must be completed. A makeup will be scheduled at a mutually agreeable time. The final exam must be written to complete the course.

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-academicrequirements-due-to-student-absence.html](https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academicrequirements-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. [https://www.dal.ca/dept/university\\_secretariat/academic-integrity.html](https://www.dal.ca/dept/university_secretariat/academic-integrity.html)

All midterms, the final exam, and written reports are to be completed individually. While student presentations are delivered individually, the class is encouraged to collaborate and provide feedback on early drafts of the presentation. Classroom discussions will be a regular feature of our lectures.

## 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 21-15 (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**

### 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](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-studentconduct.html](https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-studentconduct.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>

### 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](mailto:elders@dal.ca)).

**Information:** [https://www.dal.ca/campus\\_life/communities/indigenous.html](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](https://www.dal.ca/academics/important_dates.html)

### University Grading Practices

[https://www.dal.ca/dept/university\\_secretariat/policies/academic/grading-practices-policy.html](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](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](https://www.dal.ca/campus_life/communities/indigenous.html)

**Black Students Advising Centre:** [https://www.dal.ca/campus\\_life/communities/black-student-advising.html](https://www.dal.ca/campus_life/communities/black-student-advising.html)

**International Centre:** [https://www.dal.ca/campus\\_life/international-centre/current-students.html](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](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](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/servicessupport/student-health-and-wellness.html](https://www.dal.ca/campus_life/health-and-wellness/servicessupport/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-toget-help/ombudsperson.html](https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-toget-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>

**Dalhousie COVID-19 information and updates:** <https://www.dal.ca/covid-19-information-andupdates.html>

### A Presentation on Current Topics in Mass Spectrometry (Fall, 2021)

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). The 4206 students have the option to pre-record their talk but I want you to give yours live. 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 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 (4206 or 5206) will cover the same material. As your presentation is an integral component of this class, it is 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 in class towards the end of term (i.e. following your 2<sup>nd</sup> midterm). Your final presentation date will be selected by the instructor. Each presentation should aim to be ~35-40 min long, allowing up to 15 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 slides should be uploaded to the instructor a minimum 24 hours prior to your presentation, which will be shared with the class.

#### **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'd also like to meet with you, one-on-one. At this time, I may suggest specific content to add, emphasize or remove, and will also comments on the delivery style.



**Workshops continued:**

Your second workshop will be scheduled outside of lecture time at a mutually agreed time (up to 2 hours, minimum 1 week prior to final talk). You will outline your presentation, while also delivering a formal ‘practice talk’ for about half your presentation. The main purpose is to receive 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.

**Summary of Dates:**

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

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

Workshop 2: ~1 week prior to live 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 25 % of your total grade, with breakdown as follows:

a) Workshop #1 (rough outline)	3 marks
b) Workshop #2 (full practice)	8 marks
c) Formal presentation	14 marks

A detailed grading sheet will be provided at a later date. Note that the practice talk, presented during your second workshop, 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.**

### Written Assignment (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:**

The report is due after lectures are finished, towards the end of exam (Dec 16, 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. I will not provide any more feedback than these two drafts, and I will not accept drafts after the dates posted below.

Deadline for submission of a 1<sup>st</sup> draft: Nov 14, 2022 (5 pm)

Deadline for submission of a 2<sup>nd</sup> draft: Dec 5, 2022 (5 pm)

**Grading:**

The following breakdown will be used to assess your report. The report itself is worth 20% 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.*