Chemistry
UNIVERSITY OF TORONTO

CHM1005H: Spectroscopic Analysis in Organic Chemistry

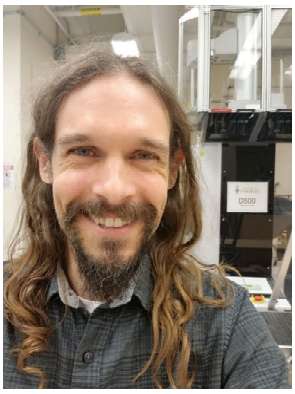
Fall 2023 Course Syllabus

I TEACHING TEAM

INSTRUCTOR (WEEKS 1 – 4)

Name: Marty Sirvinskas
Email: Martynas.sirvinskas@mail.utoronto.ca
Student hours: by appointment

INSTRUCTOR (WEEKS 5 – 12)



Name: Dr. Darcy Burns
Email: darcy.burns@utoronto.ca
Office: LM14 (CSICOMP NMR Facility)
Student hours: Tuesdays and Thursdays 11:00 AM–noon in LM14, or by appointment

TEACHING ASSISTANT

Name: Abbey Clapperton
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II COURSE OVERVIEW

COURSE DESCRIPTION:
This course will discuss the application of several spectroscopic methods available to chemistry students and researchers, including elemental analysis (EA), mass spectrometry (MS), infrared (IR) spectroscopy, and $^{1}H/^{13}C$ NMR. The fundamentals of two-dimensional NMR techniques, such as COSY and HSQC, and their importance in structural elucidation will be highlighted. Practical aspects of each method will be emphasized, and students will learn how to operate instruments pertaining to IR and NMR spectroscopy. The classes teach theory and problem-solving approaches in interpreting data to elucidate the structure of complex organic molecules. CHM1005H builds on material taught in CHM343H, CHM247H/249H, and CHM136H/CHM151Y.

We hope that you will find CHM1005H an exciting and practical course. The teaching team is here to support your learning and are invested in your success. We encourage and appreciate comments and suggestions so that we can make the course as helpful and interesting as possible. Feel free to discuss any matters with the instructors or laboratory teaching assistant.

The importance of spectroscopy cannot be overstated. Whether you work in academia or industry, proper analysis and identification of synthesized material is of paramount importance. The problem solving and analysis skills obtained by performing complex molecule structural elucidation are useful in fields beyond chemistry.

COURSE INFORMATION:
Course Times and Locations:
Lectures: Tuesdays and Thursdays, 10:10–11:00 AM, UC152 (University College, 15 King's College Circle)
Laboratory: Wednesdays, 10:10 AM–1:00 PM (only specific days in October – November, location(s) TBD)
Tutorial: Wednesday, November 1st, 10:10 AM–11:40 AM (location TBD)

COURSE WEBSITE:
Important information, including class notes, laboratory information, and test/examination information will be posted on the course website on Quercus (http://q.utoronto.ca). Please check the course website regularly for announcements and postings.

STUDENT LEARNING OUTCOMES:

Upon successful completion of the course, students will be able to:

- Use the techniques of mass spectrometry and elemental analysis to calculate the molecular mass of unknown organic molecules.
- Use the technique of infrared spectroscopy to establish which functional groups are present in an unknown organic molecule.

- Predict how an infrared vibrational frequency will change depending on the analyte structure.
- Apply the techniques of ^{1}H and ^{13}C nuclear magnetic spectroscopy to aid in the elucidation of molecular structures.
- Interpret 2D NMR spectra, including COSY, NOESY, HSQC, and HMBC.
- Utilize two-dimensional NMR to solve the atom connectivity and stereochemistry (i.e., structures) of complex organic molecules.
- Acquire 1D and 2D NMR spectra, as well as IR spectra, for the purposes of structure elucidation.
- Optimize acquisition conditions of 1D and 2D NMR experiments to provide high quality spectra for use with molecular structure elucidation.
- Report the outcomes of molecular structure analyses using standard peer-reviewed Journal formats.

PREREQUISITE COURSE(S):
This course assumes you have a basic understanding of spectroscopy content taught in CHM247H/CHM249H and CHM343H (Organic Synthesis Techniques).

READINGS:
Required: There are no required readings for this course.

Supplemental: The following texts are recommended for supplementary information and practice problems.

1) Burns and Reynolds, *Optimizing NMR Methods for Structure Elucidation*, 1st Ed., Royal Society of Chemistry, 2019
2) Silverstein, *Spectroscopic Identification of Organic Compounds*, 7th Ed., Wiley, 2005
3) Pavia, *Introduction to Spectroscopy*, 4th Ed., Brooks/Cole, 2009
4) Claridge, *High-Resolution NMR Techniques in Organic Synthesis*, 3rd Ed., Wiley, 2016

III COURSE ORGANIZATION

CHM1005H has classroom, laboratory, and tutorial instructional components. Over the course of each week, you are expected to fully participate in and attend classes. Please come prepared by having done any assigned reading and printed out in advance any class notes posted online. Questions are particularly welcomed during class.

LABORATORIES:
The laboratory component of CHM1005H will take place on certain Wednesdays during October – November. More details about the exact dates will be provided during the lectures. The laboratory component will require you to analyze an unknown sample using different spectroscopic techniques. You will be given the unknown sample, but you will prepare it for analysis yourself. The lab will showcase the importance of spectroscopic techniques in organic structure determination.

TUTORIAL:
The tutorial component of CHM1005H will take place on Wednesday, November 1st from 10:10 AM–11:40 AM. The tutorial component will provide you with an opportunity to learn about MestReNova (MNova), a program which allows you to analyze and prepare to report 1D/2D NMR data. This tutorial will provide you with an opportunity to learn many tips and tricks within MNova, enabling you to take full advantage of this program during your NMR analysis. The tutorial component will not only be useful in helping you complete the unknown lab, but also in your day-to-day analysis of NMR spectra throughout your graduate studies.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	WEEK	TOPICS
Sept. 7 – Sept. 12	1	Introduction to Mass Spectrometry and Elemental Analysis
Sept. 14 – Sept. 19	2	Introduction to Infrared Spectroscopy
Sept. 21 – Sept. 26	3	Introduction to NMR and ^{1}H NMR Spectroscopy
Sept. 28 – Oct. 3	4	Continuing ^{1}H NMR Spectroscopy and Assignment 1 given
Oct. 5 – Oct. 10	5	Introduction to ^{13}C NMR Spectroscopy
Oct. 12 – Oct. 17	6	Continuing NMR Spectroscopy, Assignment 1 due, and Midterm 1
Oct. 19 – Oct. 24	7	Nuclear Relaxation
Oct. 25	-	Unknowns Lab
Oct. 26 – Oct. 31	8	Introduction to Homonuclear 2D NMR
Nov. 1	-	MNova Processing Tutorial
Nov. 2	9a	Heteronuclear 2D NMR
Nov. 6 – 10	-	Reading week
Nov. 14	9b	Heteronuclear 2D NMR continued
Nov. 16 – Nov. 21	10	Advanced Homonuclear 2D NMR / Structure Determination, Unknowns lab due, Assignment 2 given
Nov. 23 – Nov 28	11	NMR: Special Topics
Nov. 30 – Dec. 5	12	Structure Determination, Assignment 2 due

IV EVALUATION/GRADING SCHEME

CHM1005H features two potential grading schemes. Your final grade will be calculated using the grading scheme that gives you ***the highest final overall grade***.

SCHEME 1:
Assignment 1: 12.5%
Assignment 2: 12.5%
Midterm Test: 20%
Unknowns Laboratory: 10%/15%
Oral Presentation: 10%/15%
Final Exam: 30%

SCHEME 2:
Assignment 1: 12.5%
Assignment 2: 12.5%
Midterm Test: 25%
Unknowns Laboratory: 10%/15%
Oral Presentation: 10%/15%
Final Exam: 25%

ASSESSMENT DATES & MARK BREAKDOWN:
1. Assignment 1 (12.5%, distributed on Thursday, September 28th, 2023):
Due on Thursday, October 12th, 2023, at the beginning of class.

2. Midterm Test (20/25%, Tuesday, October 17th, 2023):
50 minutes, to be written in-person during regularly scheduled class time.

3. Assignment 2 (12.5%, Tuesday, November 21st, 2023):
Due on Tuesday, December 5th, 2023.

4. Unknown Laboratory (10/15%, performed on Wednesday, October 25th, 2023):
170 minutes, to be performed during the assigned laboratory period (location TBD).
Due on Tuesday, November 21st, 2023.

5. Oral Presentation (10%/15%, due date to be determined; will be in late November):
15-minute presentations on an advanced NMR topic.

For students missing the midterm test for a valid reason, the weighting of the missed test grade will be added to the final exam.

V COURSE POLICIES

- Each member of this course is expected to maintain a:

(i) Professional and respectful attitude during all course activities, including classes, laboratories, tutorials, and online activity.
(ii) Personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
(iii) Collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation).
(iv) Familiarity with the university policy on Academic Integrity (overleaf).

- The University of Toronto is committed to equity, human rights, and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. The CHM1005H teaching team will neither condone nor

tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment, or hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.

- E-mails will generally be responded to within 48 h on weekdays. E-mails will only be accepted if: (1) You send it from your utoronto.ca email; (2) You identify the course code in the email subject, include your name, and University of Toronto student number; (3) No attachments are sent, unless official university correspondence is being forwarded (i.e. a letter detailing accommodations); (4) You are aware that chemistry, especially spectroscopy, can be talked about much more effectively through student hours rather than by emails and that sending emails is not a substitute for attending classes.
  Please only email *ONE* person on the CHM1005H instructional team, depending on the nature of your concern.

- If you are absent from your studies due to illness or other reasons and unable to complete course work (e.g., a term test or an assignment) then a piece of written documentation is required. The following four items are the recognized forms of documentation:

  1. Absence Declaration via ACORN (please note the circumstances under which an absence declaration can and cannot be submitted, and that this tool may only be used once per academic term)
  2. U of T Verification of Illness or Injury Form
  3. College Registrar's letter
  4. Letter of Academic Accommodation from Accessibility Services

  Students who complete the ACORN Absence Declaration form must additionally contact the course coordinators to discuss their situation within five business days of the missed piece of work. This is essential action for any consideration to be granted.
  For extended absences and for absences due to non-medical reasons, make sure to contact your College Registrar's Office. They can help you decide between a request for an extension or other types of academic consideration. If you suspect or know that you have a disability that is affecting your studies, learn about the services and supports available through Accessibility Services. A disability can be physical disability, sensory disability, a learning disability, mental health disorder or a short-term disability like an injury. If you are not sure whether you have a disability, you can confidentially contact Accessibility Services with your questions.

  For additional information regarding the policy on student absences, please visit Student Absences.

- The use of generative artificial intelligence tools or apps for assignments in this course, including tools like ChatGPT and other AI writing or coding assistants, is strongly discouraged. Additionally, AI tools such as ChatGPT have been shown to be ineffective in the aid of any activity associated with the field of chemistry (i.e., preparation of laboratory reports, prediction of reaction outcomes/compound spectra, etc.).

- There will be no make-up test offered. Please contact Dr. Darcy Burns immediately if you miss the term test.

  Any late assignment submissions will be subject to a deduction of 10% per day for a maximum of four days. **Please note that completed assignments will not be accepted after this period.**

  If you wish to request re-grading of any course work, please e-mail the course instructor responsible for setting the assessment.

VI INSTITUTIONAL POLICIES & SUPPORT

ACADEMIC INTEGRITY:
Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see www.academicintegrity.utoronto.ca/).

COPYRIGHT:
If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. More information regarding this is available here: https://teaching.utoronto.ca/ed-tech/audio-video/copyright-considerations/

ACCESSIBILITY NEEDS:
Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact Accessibility Services as soon as possible.

ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES:
Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor **before** the session/assignment date to arrange accommodations.

ADDITIONAL SERVICES & SUPPORT:
The following are some important links to help you with academic and/or technical service and support:

- School of Graduate Studies' Policies and Guidelines
- Full library service through University of Toronto Libraries
- Resources on academic support from the Academic Success Centre
- Learner support at the Writing Centre
- Information for Technical Support/Quercus Support
- U of T My Student Support Program (MySSP) provides students with free immediate and/or ongoing confidential, 24-hour support for any school, health, or general life concern.
- Good2Talk is a free, confidential support service for post-secondary students in Ontario. 1-866-925-5454 (Ontario); text GOOD2TALKON to 686868.

ACKNOWLEDGEMENT OF TRADITIONAL LANDS:
We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.