Chemistry
UNIVERSITY OF TORONTO

# CHM 441H/1005H: Spectroscopic Analysis in Organic Chemistry

**Fall 2021 Course Syllabus**

## I TEACHING TEAM

**INSTRUCTOR (WEEKS 1 – 6)**

Name: Bijan Mirabi
Email: bijan.mirabi@mail.utoronto.ca

Student hours: Tuesdays and Thursdays 11 a.m. – 12 noon, or by appointment

**INSTRUCTOR (WEEKS 7 – 12)**

Name: Dr. Darcy Burns
Email: darcy.burns@ utoronto.ca
Office: LM14 (CSICOMP NMR Facility)
Student hours: Tuesdays and Thursdays 11 a.m – 12 noon in LM14, or by appointment

## II COURSE OVERVIEW

**COURSE DESCRIPTION:**

This course will discuss the application of several spectroscopic methods available to chemistry students and researchers, including mass spectrometry (MS), infrared (IR), $^{1}H$, and $^{13}C$ 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. The classes teach theory and problem-solving approaches in interpreting data to elucidate the structure of complex organic molecules. CHM441H/1005H builds on material taught in CHM343H, CHM247H/249H, and CHM136H/CHM151Y.

We hope that you will find CHM441H/1005H 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

Classes: Tuesdays and Thursdays 10:00 – 11:00 a.m. in LM 157 (Lash Miller Chemical Laboratories, 80 St. George Street)
Laboratory: Wednesdays 10 – 1 a.m. in LM 217 or LM 121 (only specific days in October – November)

**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 vibration 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 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
- Use density functional theory to compute IR and NMR parameters of organic molecules and use the outcomes to verify molecular structures
- 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). CHM343H is a pre-requisite course for CHM441H.

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

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

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

## III COURSE ORGANIZATION

CHM441H/1005H has both class and laboratory instructional components. The classes for the first two weeks will be delivered completely online during the Fall 2021 semester. The rest of the classes will be conducted in person (unless otherwise mandated by the university). 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 CHM441H/1005H will take place on certain Wednesdays during October – November. More details about the exact dates will be provided in due course. The laboratory component includes a computational lab that will be run by Dr. Mima Staikova. There is also a 'wet' lab component that 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 labs will showcase the importance of computational and spectroscopic techniques in organic structure determination.

**COURSE SCHEDULE & RELEVANT SESSIONAL DATES:**

| DATES | WEEK | TOPICS |
|---|---|---|
| Sept. 9 – Sept. 14 | 1 | Introduction to Mass Spectrometry and Elemental Analysis |
| Sept. 16 – Sept. 21 | 2 | Introduction to Infrared Spectroscopy |
| Sept. 23 – Sept. 28 | 3 | Introduction to NMR and $^{1}$H NMR Spectroscopy |
| Sept. 30 – Oct. 5 | 4 | Continuing $^{1}$H NMR Spectroscopy and Assignment 1 given |
| Oct. 7 – Oct. 12 | 5 | Introduction to $^{13}$C NMR Spectroscopy |
| Oct. 14 – Oct. 19 | 6 | Continuing NMR Spectroscopy, Assignment 1 due, and Midterm 1 |

| | | |
|---|---|---|
| Oct. 21 – Oct. 26 | 7 | Nuclear Relaxation and Introduction to 2D NMR |
| Oct. 28 – Nov. 2 | 8 | Advanced Homonuclear NMR |
| Nov. 4 | 9 | Practical Lecture – Being an NMR Spectroscopist |
| Reading week / Nov. 16 | 10 | Heteronuclear 2D NMR and Assignment 2 given |
| Nov. 18 – Nov. 23 | 11 | Continuing Heteronuclear 2D NMR and Structure Elucidation |
| Nov. 30 – Dec. 2 | 12 | Continuing 2D NMR and Assignment 2 due |

## IV EVALUATION/GRADING SCHEME

CHM441H/1005H 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: 10%
Assignment 2: 10%
Computational Laboratory: 5%
Midterm Test: 25%
Unknowns Laboratory: 15%
Final Exam: 35%

**SCHEME 2:**
Assignment 1: 10%
Assignment 2: 10%
Computational Laboratory: 5%
Midterm Test: 30%
Unknowns Laboratory: 15%
Final Exam: 30%

**ASSESSMENT DATES & MARK BREAKDOWN:**
1. Assignment 1 (10%, distributed on Thursday, September 30th, 2021): Due on Thursday, October 14th, 2021 at the beginning of class.

2. Midterm Test (25/30%, Tuesday, October 19th, 2021): 50 minutes, to be written in-person during regularly scheduled class time. Synchronous "debrief" session to be held on Tuesday, October 26th, 2021 from 8–10 p.m. through Zoom. This session is not mandatory to attend.

3. Computational Laboratory (5%, performed on Wednesday, October 13th, 2021): 170 minutes, to be performed during the assigned laboratory period. The computational lab will be performed remotely. The instructions on how to access the computational cluster and how to perform the calculations will be posted on the Quercus class site. There will be a Zoom session offered on October 13th where you

will finalize your calculations and discuss the lab report with the Computational Lab instructor, Dr. Staikova. Report due in class on Tuesday, November 2nd, 2021.

4. Assignment 2 (10%, Tuesday, November 16th, 2021): Due on Tuesday, December 7th, 2021.

5. Unknowns Laboratory (15%, performed on Wednesday, October 20th, 2021): 170 minutes, to be performed during the assigned laboratory period. Due on Tuesday, November 16th, 2021

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. As course instructors, we 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 CHM441H/1005H instructional team, depending on the nature of your concern.**

- 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.**

- There will be no make-up test offered. Please contact Bijan Mirabi immediately if you miss the term test.

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

## VI TECHNOLOGY REQUIREMENTS

- Most of the course will be held in-person. Please view specific guidance from the U of T Vice-Provost, Students regarding student technology requirements here: https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/

- Advice for students more broadly regarding online learning is available here: https://onlinelearning.utoronto.ca/getting-ready-for-online/

- This course requires the use of computers, and technical issues are possible. When working on a piece of academic work, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date independent backup copy of your work is strongly recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

## VII 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 (governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In laboratory reports:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any report. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post virtual laboratory report material/questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**

On term tests:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post quiz/term test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**
2. Looking at someone else's answers or collaborating/discussing answers during a term test.
3. Misrepresenting your identity.

In general academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

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:**

Parts of this course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session. Course videos and materials belong to your instructor, the University, and/or other source depending the specific facts of each situation, and are protected by copyright. In this course, you are permitted to download session videos and materials for your own academic use, but you should not copy, share, or use them for any other purpose without explicit permission of the instructor. For questions about recording and use of videos in which you appear, please contact your instructor.

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:

- General student services and resources at Student Life
- Full library service through University of Toronto Libraries
- Resources on conducting online research through University Libraries Research
- Resources on academic support from the Academic Success Centre
- Learner support at the Writing Centre
- Information for Technical Support/Quercus Support

**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.