Chemistry
UNIVERSITY OF TORONTO

CHM 1005H: SPECTROSCOPIC ANALYSIS IN ORGANIC CHEMISTRY

Fall 2024 Course Syllabus

I TEACHING TEAM

INSTRUCTOR (Weeks 1-6) AND LABORATORY COORDINATOR
Name: Professor Kylie Luska
Email: kylie.luska@utoronto.ca
Research: https://www.chemistry.utoronto.ca/people/directories/all-faculty/kylie-luska
Office: Lash Miller: LM 219
Student hours: Tuesday and Thursday 11:00 AM – 12:00 PM

INSTRUCTOR (Weeks 7-12)
Name: Dr. Darcy Burns
Email: darcy.burns@utoronto.ca
Office: Lash Miller: LM 14
Student hours: Tuesday and Thursday 11:00 AM – 12:00 PM

TEACHING ASSISTANT
Name: Abbey Clapperton
Email: Abigail.clapperton@mail.utoronto.ca

COMPONENT COURSE SUMMARY

LECTURES	**Tuesday and Thursday (weekly starting September 3rd)** 10:00 AM – 11:00 AM UC 87
LABORATORIES	**Wednesday (only selected weeks in Oct. and Nov.)** 10:00 AM – 1:00 PM LM 217

II COURSE OVERVIEW

A very warm welcome to CHM1005H! This course will discuss the application of spectrometric and spectroscopic techniques used to analyze and determine the structures of organic compounds including: mass spectrometry (MS), infrared spectroscopy (IR), and nuclear magnetic resonance spectroscopy (NMR). The course will advance the understanding and application of MS, IR and one-dimensional NMR techniques. The theoretical background and application of two-dimensional NMR techniques will be presented including: homonuclear $^{1}H–^{1}H$ correlations (*e.g.*, COSY, NOESY) and heteronuclear $^{1}H–^{13}C$ correlations (*e.g.*, HSQC, HMBC). The classes teach theory and problem-solving approaches in interpreting data to elucidate the structure of complex organic molecules. The laboratory teaches students to operate various instruments and understand the practical aspects of each method. CHM1005H builds on material taught in CHM343H, CHM247H/249H, and CHM136H/CHM151Y.

We sincerely hope that CHM1005H will exceed your expectations: we are all here to support your learning and are very invested in your success! We would appreciate your comments and suggestions so that we can make the course as helpful and interesting as possible. Do feel free to discuss any matters with Professor Luska, Dr. Burns and the laboratory teaching assistants (TAs).

STUDENT LEARNING OUTCOMES

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

- Use the techniques of elemental analysis and mass spectrometry to calculate the molecular mass of organic compounds
- Employ the technique of mass spectrometry to predict the presence of heteroatoms and various functional groups based on fragmentation patterns
- Utilize the technique of infrared spectroscopy to identify various functional groups and predict how infrared vibrations change depending on the analyte structure
- Apply the techniques of ^{1}H and ^{13}C nuclear magnetic spectroscopy towards the analysis and elucidation of organic structures
- Describe the theoretical background for two-dimensional NMR techniques
- Use homonuclear $^{1}H–^{1}H$ correlations (*e.g.*, COSY, NOESY) and heteronuclear $^{1}H–^{13}C$ (*e.g.*, HSQC, HMBC) two-dimensional NMR techniques to elucidate complex organic structures
- Prepare samples for various spectrometric and spectroscopic techniques
- Acquire and process 1D and 2D NMR spectra for the purposes of structure elucidation
- Report the outcomes of molecular structure analyses using standard peer-reviewed journal formats

PREREQUISITE COURSES

This course assumes you have a basic understanding of the spectroscopy content taught in CHM136H/CHM151Y and CHM247H/CHM249H.

REFERENCE MATERIAL

Required – There are no required texts for this course.

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

1. *Spectroscopic Identification of Organic Compounds*, 8th edition by R. M. Silverstein, F. X. Webster, D. J. Kiemle and D. L. Bryce, Wiley, 2015.
2. *Optimizing NMR Methods for Structure Elucidation*, 1st edition by D. C. Burns and W. F. Reynolds, Royal Society of Chemistry, 2019.
3. *High-Resolution NMR Techniques in Organic Synthesis*, 3rd edition by T. D. W. Claridge, Wiley, 2016.
4. *Introduction to Spectroscopy* – 5th edition by *D. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan*, Cengage, 2015.

III HOW THE COURSE IS ORGANIZED

OVERVIEW
CHM1005H has two instructional components – classes and laboratories. **As per the Faculty of Arts & Science timetable, all instruction will be delivered in-person as of Tuesday September 3rd.** An announcement will be made if the delivery mode of any or all instructional components needs to change for any reason.

CLASSES
Classes will be offered in-person ONLY throughout the semester on Tuesday and Thursday from 10:00–11:00 AM in University College, room UC 87. Please come prepared to class with a print or electronic copy of the class notes posted on Quercus. Questions are particularly welcomed both during class time and after class. Do be aware that reading the posted class notes and/or textbook is not a substitute for attending classes and taking an active approach to your learning! It is essential that you attend class in-person in order to solidify your understanding of the fundamental course material.

A list of planned topics that will be covered in class is as follows:

- Determination of molecular formula
- Mass spectrometry
- IR spectroscopy
- 1D NMR (including ^{1}H, ^{13}C, ^{19}F and ^{31}P)
- NMR theory
- Homo- and heteronuclear 2D NMR (including COSY, NOESY, HSQC and HMBC)

LABORATORIES
The laboratory component of CHM1005H will take place on certain Wednesdays from 10:00 AM – 1:00 PM during October and November. The laboratory will allow you to gain hands-on experience related to sample preparation, data acquisition and spectral processing for various spectroscopic techniques.

IMPORTANT FALL 2024 SESSIONAL DATES:
First Day of S classes: Tuesday September 3rd, 2024
Thanksgiving (no classes): Monday October 14th, 2024
Fall Reading Week (no classes): Monday October 28th to November 1st, 2024
Last Day to Drop F Courses: Monday November 4th, 2024

Last Day of F classes: Monday December 2nd, 2024
Study Days: December 4th and 5th, 2024
Final Exam Period: December 6th to 21st

IV EVALUATION/GRADING SCHEME

OVERVIEW:
Your overall course grade is based on your performance in the laboratory, in one term test, in two assignments, in an oral presentation and in a final examination. CHM1005H features four 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%
Laboratory = 15%
Oral Presentation = 10%
Term Test = 20%
Final Exam = 30%

SCHEME 2
Assignment 1 = 12.5%
Assignment 2 = 12.5%
Laboratory = 10%
Oral Presentation = 15%
Term Test = 20%
Final Exam = 30%

SCHEME 3
Assignment 1 = 12.5%
Assignment 2 = 12.5%
Laboratory = 15%
Oral Presentation = 10%
Term Test = 25%
Final Exam = 25%

SCHEME 4
Assignment 1 = 12.5%
Assignment 2 = 12.5%
Laboratory = 10%
Oral Presentation = 15%
Term Test = 25%
Final Exam = 25%

ASSIGNMENTS

Assignments will allow you to stay up-to-date with the course material and aid in the development of the problem-solving skills needed to analyze and elucidate organic structures using spectrometry and spectroscopy. Assignments will be released and submitted according to the following schedule:

Assignment 1 (12.5%) — Release Date – Thursday September 26th; Due Date – Thursday October 10th at 11:45 PM

Assignment 2 (12.5%) — Release Date – Thursday November 14th; Due Date – Monday December 2nd at 11:45 PM

Completed assignments will be submitted to Crowdmark for grading. A late penalty of 10% per day will be applied to assignments submitted after their due date. Late assignments will ONLY be accepted up to THREE DAYS LATE, after which they will not be graded. This policy will allow for solutions for the assignments to be posted to Quercus in a timely manner to aid in the preparation for examinations.

You are responsible for completing the assignments on YOUR OWN! Solutions CANNOT be completed within a group collaboration, obtained from an online tutor website or copied from posts within a group chat (see below for further information on the University of Toronto's Code of Behaviour on Academic Matters)! If you do not attempt these assignments on your own, then you are not giving yourself a chance to identify your strengths and weaknesses in the course material and as such will be unsure what topics to focus on to succeed on the exams.

LABORATORIES

The lab component involves the analysis of an unknown organic compound using different spectroscopic techniques. In the lab, you will be responsible for preparing your sample for each technique, acquiring spectra and processing your spectral data. Outside of the lab, you will interpret your spectral data to determine the molecular structure of your unknown compound and report your data using standard peer-reviewed journal formats.

Data Acquisition Wednesday October 23rd (during lab time)
Report Due Date (15 or 10%) Monday November 25th at 11:45 PM (submitted to Crowdmark)

ORAL PRESENTATION
(10 or 15%)

The oral presentation involves research and presentation on an advanced NMR topic. Presentations will take place towards the end of the term.

EXAMINATIONS

Term Test (20 or 25%) — Wednesday October 16th (during lab time); 10:00 AM –12:00 PM (120 minutes)

Final Exam (30 or 25%) — Scheduled by the Faculty of Arts and Science; 180 minutes

There is no make-up test in CHM 1005H. If you are absent from your studies due to illness or other reasons and are unable to complete the term test, then a piece of written documentation is required (see below for further information).

Information Regarding Use of Artificial Intelligence Tools in the Writing of Laboratory Reports and Assignments:

Generative Artificial Intelligence (AI) technology is evolving quickly, and it is necessary to specifically address this within the context of CHM1005H lab reports and assignments. AI tools such as ChatGPT (GPT stands for Generative Pre-trained Transformer) are large language models that have been trained on a limited dataset to generated content based on prompts and the data it has been trained on. **It is important to recognize there are major limitations to these tools, particularly in more specialized subjects such as chemistry.** Currently, ChatGPT and many similar models are only trained on freely available data and will not include information that is only accessible through payment, which includes much of the scholarly literature, textbooks, etc. (There is a lot of reliable information on the internet, but there is also a lot of junk, and ChatGPT does not know how to tell the difference: it has no concept whatsoever of scientific accuracy). In addition, ChatGPT does not cite its sources: when asked to include citations, it will routinely reference papers that do not exist. By using ChatGPT to generate text, you run the risk of accidentally plagiarizing one of the many sources that are included as part of its training data.

Important learning outcomes for CHM1005H are: (i) development of effective scientific communication skills; and (ii) interpretation of spectral data towards the elucidate of chemical structures. The practice and repetition of writing on your own has been shown in numerous scientific reports to lead to deeper and longer lasting learning. *In this course, the use of ChatGPT and/or other generative AI tools is permitted within the limitations of reviewing your own written work for additional suggestions of grammar, punctuation, etc*. In this manner, the tool is educational and can help you develop better writing skills when used critically and for self-analysis. **However, it is both ill-advised and prohibited to solely use these tools to attempt to write or analyze components of formal laboratory reports.** As mentioned previously, the capabilities of the systems are limited, and you will not develop the scientific communications skills needed for future studies or careers. **In summary, it is well established that these tools will misuse and fabricate information and referencing, which will be noticeable by your TAs and laboratory instructors and will leave you susceptible to academic discipline violations (see below for further information).**

V IMPORTANT COURSE POLICIES

- Each member of this course is expected to maintain a:
  - professional and respectful attitude during all course components, including classes, laboratories, assessments and any online activity
  - personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met
  - 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)
  - familiarity with the university policy on Academic Integrity (overleaf)

- Course website: q.utoronto.ca. **Please check the Quercus course website regularly for**:
    - general course information
    - class notes
    - laboratory information
    - all important announcements related to class, laboratories and assessments

- Email will generally be responded to within 24 hours on weekdays. Email will only be accepted if: (1) You send it from your utoronto.ca account; (2) You identify yourself in the email subject as a student in CHM 1005H and include your name and University of Toronto student ID number; (3) No attachments are sent, unless official university correspondence is being forwarded (*e.g.*, a letter detailing academic accommodations or an ACORN absence declaration); and (4) You are aware that spectral data can be talked about much more effectively through student hours rather than by email, and that sending emails is not a substitute for attending classes. The finalized student hours for each instructor are posted at the top of the syllabus and they are additionally available by appointment.

Important: be sure to email only ONE person within the CHM 1005H instructional team, depending on the nature of your concern. Please do not send emails through the Quercus internal email system (they will not be responded to): the contact information for the course instructor/laboratory coordinator/teaching assistants is listed at the top of the syllabus.

- 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 members of the course teaching team, we will not 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 and 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.

- Students may not create audio or video recordings of classes except for those students requiring an accommodation for a disability, who should contact the instructor prior to beginning to record classes for written permission. Students creating unauthorized audio recording of classes violate an instructor's intellectual property rights and the Canadian Copyright Act. Students violating this agreement will be subject to disciplinary actions under the Code of Student Conduct.

- Assignments and laboratory reports are to be submitted through the CHM 1005H Crowdmark site only. Late assignments and reports will be deducted at 10% per day to a maximum of three days, **after which they will not be graded**.

There is no make-up test in CHM 1005H, and there are no make-up laboratory sessions. If you are absent from your studies due to illness or other reasons and are unable to complete course work (*e.g.*, a term test or a laboratory report) 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)

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 and miss a term test or laboratory session must additionally contact the instructor and laboratory coordinator, Professor Kylie Luska (kylie.luska@utoronto.ca) to discuss their situation within five business days of the missed activity. 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.

VI TECHNOLOGY REQUIREMENTS

- This course requires the use of computers, and technical issues are possible. When working on a piece of work such as a laboratory report, 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 occurrences such as hard-drive failures, corrupted files, lost computers, etc. *We encourage you to spend a moment at the start of the semester to plan for what you would do if you lost access to the computer that you primarily intend to use, which will help ensure that you are prepared for this unlikely possibility.*

VII INSTITUTIONAL POLICIES AND 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. Potential offences include, but are not limited to:

In assignments/laboratory reports:
- using someone else's ideas or words without appropriate acknowledgement
- submitting your own work in more than one course without the permission of the instructor
- making up sources or facts
- obtaining or providing unauthorized assistance on any report. **Please note that the use of websites (such as Chegg.com) to post assignment/laboratory report 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:
- using or possessing unauthorized aids.
- looking at someone else's answers or collaborating/discussing answers during a term test.
- misrepresenting your identity.

In general academic work:
- falsifying institutional documents or grades.
- 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).

PLAGIARISM DETECTION

Normally, students will be required to submit their course essays and tests to the University's plagiarism detection tool for a review of textual similarity and detection of possible plagiarism. In doing so, students will allow their work to be included as source documents in the tool's reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of this tool are described on the Centre for Teaching Support & Innovation web site: https://uoft.me/pdt-faq.

ACCESSIBILITY NEEDS

Students with diverse learning styles and needs are welcome in CHM 1005H. 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. If possible, please submit your accessibility letter at the beginning of the course and not immediately before laboratory report or assignment is due.

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, class or laboratory session. Students must inform the instructor **before** the 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.