

**CONCORDIA UNIVERSITY
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

**CHEM 498-51/620-51
NONCOVALENT INTERACTIONS**

SYLLABUS – Fall 2019

GENERAL INFORMATION

Noncovalent Interactions is an advanced course in modern Physical Organic Chemistry. Prerequisites are a solid foundation in organic chemistry (CHEM 324 or CHEM 325) and organic spectroscopy (CHEM 293). A basic knowledge in computational chemistry as provided through CHEM 325 or CHEM 293 is sufficient. The material covered is applicable in chemistry and biochemistry alike.

INSTRUCTOR	Professor H.M. Muchall Office LOY SP 275.15 Tel. (514) 848-2424 x3342 (I will not return calls.) heidi.muchall@concordia.ca
COURSE FORMAT	Lectures and computer labs
LECTURE HOURS	Monday 18:00 – 20:30
LOCATION	LOY CC 425
COURSE WEBSITE	on Moodle: CHEM 498 NCI 51, CHEM 620 2192
OFFICE HOURS	Tu 15:00 – 16:00 Plus: drop-in “anytime”: just come on in if I’m in the office!

LECTURES AND READING

There is no single textbook for this advanced course. A list of textbooks that are available in the library, some of which have been put on reserve, or online is suggested on the course website.

COURSE OBJECTIVES

- To raise the awareness of the occurrence of noncovalent interactions in (organic) chemistry.
- To provide knowledge of selected experimental tools for the analyses of noncovalent interactions.
- To enable students to identify noncovalent interactions using selected computational tools.

COURSE OUTLINE

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|--------|---|
| Part 1 | Introduction to “structure” |
| Part 2 | Use of electronic structure calculations and the electron density |
| Part 3 | Use of IR spectroscopy |
| Part 4 | Use of NMR spectroscopy |
| Part 5 | Use of X-ray and neutron diffraction |
| Part 6 | Selected problems that can arise |

Links to the lecture slides (as pdf) can be found on the course website. The slides are posted for you to print and bring to class to annotate; they are not meant as stand-alone material. A more detailed description of each topic is provided as slide 1 within each link.

COMPUTER LABS

Four (4) lecture periods (followed by an additional hour should a student need to use it) are set aside for practical work in the computer lab (SP S-185.07). You will learn how to generate and use computational data to identify and analyze noncovalent interactions in small model systems. The lab manual can be found on the course website.

Short lab reports that focus on data analysis and interpretation are required. For selected labs, a reading sample will be provided in advance, and questions on it must be answered in the lab report. A sample report is posted on the course website.

Attendance is mandatory. If you are absent from the lab, you must produce a written excuse appropriately signed (i.e., by a doctor or an employer) on the appropriate letterhead paper. This letter must be delivered to the instructor (me) as soon as possible but **no later than one week** after the missed lab. The Department determines the validity of the absence. If there is no valid excuse, you will receive a mark of zero for the lab report. In case of a valid absence, the percentage will be added to that of the exam. You will then be responsible for acquiring the skills yourself: do the lab in your spare time.

EXAMINATION

There will be one (1) formal examination, in SP S-185.07, on

December 2, 2019.

Permission to have the exam on the last regular day of classes was obtained.

The exam is designed to test your practical and theoretical knowledge: you will generate computational data on a given problem and interpret your results in answering posed questions.

If you are absent from the exam, you must produce a written excuse appropriately signed (i.e., by a doctor or an employer) on the appropriate letterhead paper. This letter must be delivered to the instructor (me) as soon as possible but **no later than December 6, 2019**. The Department determines the validity of the absence. If there is no valid excuse, you will receive a mark of zero for the exam. In case of a valid absence, a make-up exam will be offered.

ACADEMIC HONESTY (Source: <http://www.concordia.ca/students/academic-integrity.html>)

Go to the link above and familiarize yourself with what you are supposed to do and what you are supposed to avoid doing.

The most common offense under the Academic Code of Conduct is plagiarism, which the Code defines as “the presentation of the work of another person as one's own or without proper acknowledgement.”

“Work” here could be material copied word for word from books, journals, internet sites, professor's course notes, etc. It could be material for which the words have been changed but whose phrasing still closely resembles that of the original source. It could be the work of a fellow student, e.g., a lab report completed by another student, or unauthorized data for a lab report. It could be a paper purchased through one of the many available sources. “Plagiarism” does not refer to words alone – it also refers to images, graphs, tables and ideas. “Presentation” is not limited to written work. It also includes computer and artistic works. Finally, if you translate the work of another person into English and do not cite the source, this is also plagiarism.

The Academic Code of Conduct can be found at <http://www.concordia.ca/students/academic-integrity.html> and in the undergraduate calendar (<http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html>). Any form of cheating, unauthorized collaboration, copying or plagiarism found in this course will be reported and the appropriate sanctions applied.

As part of CHEM 498/620-51, you are **required** to attend a seminar and pass a quiz on avoiding plagiarism and other forms of academic dishonesty, offered by the Department of Chemistry and Biochemistry. If you have already attended the seminar and achieved 100 % (110 points) on the quiz **within the past five (5) years (i.e. Fall 2014 or more recently)**, you have fulfilled the requirement. The aim of the seminar and quiz is to clarify which practices are considered unacceptable by the Department of Chemistry and Biochemistry. The seminar will be offered during the third week of classes (see the appendix for the times offered); the quiz is online, can be accessed through the MyConcordia portal (click on Powered by Moodle under Course Websites and choose CHEM 101 under Specialized Chemistry Sites) and can be taken from after the seminar up to the deadline announced on the CHEM 101 site, but preferably as soon as possible. **If you do not attend the seminar and/or do not pass the quiz (the passing mark is 100 %), your grade will be lowered by one full letter grade with an incomplete (INC) notation.** Please refer to the academic calendar section 16.3.5

(<http://www.concordia.ca/academics/undergraduate/calendar/current/sec16/16.html#b16.3.5>) on how to remove the INC and restore the proper grade.

COURSE GRADE

The final grade of the course is based on the marks obtained in the reports and the exam. The composition of the final course grade is as follows:

Lab Reports (4)	60 % (15% each)
Exam	40 %

The grading scales (percentage to letter grade) follow (normal rounding applies):

	UGrad CHEM 498	Grad CHEM 620
100-90	A+	A+
89-85	A	A
84-80	A-	A-
79-77	B+	B+
76-73	B	B
72-70	B-	B-
69-67	C+	C
66-63	C	
62-60	C-	
59-57	D+	F
56-53	D	
52-50	D-	
<50	FNS	

FNS grade: for this failing grade, a supplemental exam is not available. For graduate students, C and F rules (<http://www.concordia.ca/academics/graduate/calendar/current/academic-regulations.html>) apply.

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

H.M. Muchall, August 2019

Appendix

Seminar on academic conduct

Date (Fall 2019)	Time	Room
Monday, Sept. 16	16:45-17:45	CC 111
Tuesday, Sept. 17	16:45-17:45	CC 308
Tuesday, Sept. 17	20:45-21:45	HB 130
Wednesday, Sept. 18	16:45-17:45	CC 308
Wednesday, Sept. 18	20:45-21:45	HB 130
Thursday, Sept. 19	16:45-17:45	HC 155
Friday, Sept. 20	16:45-17:45	HC 157

As space for each of the seminars is limited by the room size, please sign up to your preferred time. Sign-up sheets are available outside SP 201-01 (Departmental office).