UNIVERSITY OF CALGARY

UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2021

1. **Course:** CHEM 659.28, Selected Topics in Organic Chemistry (Molecular Structure and Reactivity)
Lecture Section: L01
DATE/TIME MWF 15:00-15:50, F 14:00-14:50 on weeks when there is a conflict with departmental seminar WEB BASED, Dr. Van Humbeck (jeffrey.vanhumbec1@ucalgary.ca)
Office hours: By appointment

Chemistry Department Office: Science A 229, 403.220.5341, chem.info@ucalgary.ca

It is recommended that students use their U of C account for all correspondences.

D2L: CHEM 659 L01 - Selected Topics in Organic Chemistry

2. **Course Description**
In this course, students will be introduced to modern methods of experimental design and analysis that are highly relevant to experimental chemistry as practiced in research labs today. To achieve this goal three specific skills will be delivered, which reflect the division of the course into three units. The dates of unit exams will not change, but all other dates are subject to change.

(i) Machine Learning in Chemistry (No Unit Exam)
First, students will be introduced to 'machine learning' (ML) as a tool for both data analysis and predictive modelling. It is assumed that students have no background in this area, and none will be required to be successful in the class. With some basic understanding, students will be asked to find an open-source ML tool that could be useful to their research group. The last 4 classes of the semester will consist of the students giving a brief presentation on the technique they discovered. A second ML-focused component will occur throughout the semester, where small groups will work together to design a novel organic molecule for a pharmaceutical target using ML tools, to learn their strengths and limitations.

January 11: Introduction – how do machines learn from data?
January 13: Major types of machine learning
January 15: The basic components of a neural network
January 18: 'Inductive bias' and convolutional neural networks
February 11: First molecule design submission due
March 1: Second molecule design submission due
March 19: Final molecule design submission due (grade is assigned at this submission)
March 24, 26, 29: Modern applications of machine learning in chemistry
April 7, 9, 12, 14: Student presentations

*(ii) Theoretical tools for understanding experimental design (**Unit 2 Exam: February 24, 2021**)*

In the second unit, students will be introduced to improved theories of bonding and reactivity so that it is possible to understand the more advanced experimental designs introduced in the final section of the course.

January 20: What is a “reaction coordinate” (really)?
January 22: Three-dimensional reaction surfaces and MOJ plots
January 25, 27: Transition state theory and the Hammond postulate
January 29: How many “types” of electrons are there in methane?
February 1, 3: Qualitative molecular orbital theory (QMOT)
February 5: Important results of energy level alignment: reaction vs. electron transfer
February 8: Proton-coupled electron transfer
February 10, 12: Non-covalent forces

*(iii) Experimental design strategies (**Unit 3 Exam: March 31, 2021**)*

In the final unit, the experimental designs introduced will be both single experiments that are used to understand a reaction better (such as kinetic isotope effects), or campaigns of related reactions used to improve the performance of a new process (such as the ‘PHOENICS’ approach). By the end of course, students will be prepared to propose well-designed experiments that will be useful when they are engaged in modern laboratory work.

February 26, March 1, 3, 5: Kinetic isotope effects, labelling, and crossover experiments
March 8, 10, 12: Linear-free energy investigations and multivariate experiments
March 15: The ‘Design-of-Experiment’ (DoE) approach in chemistry
March 17, 19: Better-than-DoE design in chemistry

3. Graded Components and Description

Grades will be assigned based on unit exams (Unit 2: 25%, Unit 3: 25%), the final presentation (25%), and the work submitted towards novel molecule design (25%). Detailed descriptions of the grading rubric for the presentation and molecule design components will be provided on D2L by the end of the first day of lecture.

ALL OTHER CRITICAL COURSE INFORMATION CAN BE FOUND ON THE OFFICIAL COURSE INFORMATION SHEET