Faculty of Engineering and Applied Science

CHEE 324 – ORGANIC PROCESS DEVELOPMENT

Course Syllabus – Winter 2022

This is your course syllabus. Please download the file and keep it for future reference.

TEACHING TEAM

COURSE INSTRUCTOR

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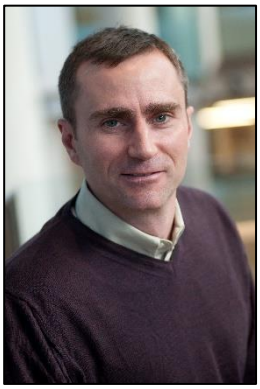

Please check the course website for an up-to-date list of TAs and other course personnel.

COURSE INFORMATION

COURSE DESCRIPTION

Students will expand their knowledge of functional group interconversions and C-C bond forming reactions learned in ENCH 245, and apply retrosynthetic analysis to propose multi-step syntheses of organic target molecules. Selection of reagents, solvents and reaction conditions will be examined in the context of process safety, reaction yield, product isolation, and profitability. This will be followed by studies of target molecule recovery by extraction, recrystallization, distillation and chromatography.

The design component of the course involves the development of a complete process for preparing an active pharmaceutical ingredient based on established syntheses in the scholarly and patent literature. Students will work in pairs to adapt these syntheses to improve health and safety, economics, and operability, including changes to process chemistry and product isolation techniques.

Prerequisites: ENCH 245 and CHEE 311; no co-requisites or exclusions

COURSE LEARNING OUTCOMES (CLO)

By the end of this course, students will be able to:

CLO	DESCRIPTION
CLO 1	Devise multistep reaction sequences leading to the synthesis of organic molecules containing up to three functional groups
CLO 2	Adapt organic syntheses taken from the scholarly and patent literature to improve process safety, environmental impact, economics and operability
CLO 3	Devise methodologies for quenching reaction mixtures and isolating target molecules, including appropriate use of liquid-liquid extraction, distillation, chromatography, recrystallization and trituration
CLO 4	Summarize multi-step organic processes using appropriate block flow diagrams

RELEVANCE TO THE PROGRAM

This engineering science and design course covers strategies for synthesizing fine chemicals by environmentally-responsible and economically-viable methodologies, which is a fundamental topic of the Process Synthesis design pillar of the Engineering Chemistry program. The course assumes knowledge of 2nd year Organic Chemistry and 3rd year Phase and Reaction Equilibrium, and requires general applications of engineering and mathematical tools taught in previous years of study. These principles are applied in the 4th year design course, CHEE 471 – Chemical Process Design.

Course Structure and Activities

3 lecture hours + 1 tutorial hour per week. Please refer to SOLUS for times and locations.

Expectations for Lectures/Tutorials

Lecture slides will be posted in advance through the onQ learning environment. These course notes are incomplete, and lectures will include examples and problem solutions not contained in the posted slides. Students are expected to read associated sections and study worked examples provided in the textbook and online. Self-study problem sets are available for each lecture, with solutions posted online. These must be completed as soon as each topic has been discussed in class. It is strongly recommended that each student attempts all the suggested problems, as they are selected to help practice the analytical tools provided in class.

Course Materials

Recommended Textbook

"Organic Chemistry" 2nd Ed., by Clayden, Greeves, Warren is available from the campus bookstore in hard copy. The textbook is listed as mandatory for the prerequisite course, ENCH 245 and extensive use of the textbook is made throughout the term, including reference to numerous tables and appendices. Previous editions may be used; however contents may not match references listed in course material.

Other Material

All other course material is accessible via OnQ.

Course Evaluation

Deliverable	Week or Date	Weight
Fundamental Review Quiz	Weeks 2	10%
Design Project		20%
Midterm Exam	Week 8	20%
Design Challenges		15%
Final Exam	Exam period	35%

Assigned Problems: Problem sets will be provided throughout the term to illustrate key principles. Only some problems will be marked, but it is essential that all exercises be completed. Skeletal solutions to these problems will be presented in tutorial sessions to allow students to monitor their progress.

Design Exercises: Several group design challenges will be undertaken, each illustrating a main principle of the course. **Attendance at these sessions is mandatory, and students will be assigned a mark of zero if they do not complete an exercise, as dictated by departmental policy.**

All assessments in this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to the established Grade Point Index.

Unless other arrangements have been approved, departmental policies regarding late and missed assignments, and missed quizzes/exams will be followed. Only a Casio 991 non-programmable, non-communicating calculator will be allowed during tests and exams.

COURSE POLICIES

Please review the following policies concerning copyright, academic integrity, absences and academic accommodations:

COPYRIGHT

Unless otherwise stated, the material on the course website is copyrighted and is for the sole use of students registered in this course. The material on the website may be downloaded for a registered student's personal use but shall not be distributed or disseminated to anyone other than students registered in this course.

ACADEMIC INTEGRITY

Information on policies concerning academic integrity is available in the Queen's University Code of Conduct, in the Senate Academic Integrity Policy Statement, on the Faculty of Engineering and Applied Science website, and from your instructor.

ABSENCES (ACADEMIC CONSIDERATION) AND ACADEMIC ACCOMMODATIONS

For absences and academic accommodations please review the information on the FEAS website.

TECHNICAL SUPPORT

No specialized computer-related technical skills are required for this course. If you require technical assistance, please contact Technical Support.

PERSONAL SUPPORTIVE COUNSELLING

If at any time you find yourself feeling overwhelmed, anxious, sad, lonely, or distressed, consider confidential supportive counselling offered by the Faculty of Engineering and Applied Science.

Course Outline

Part 1: Review and Expansion of Functional Group Interconversions:
- functionalization of alkanes
- functionalization of isolated and conjugated alkenes
- transformations of alkynes, aromatic hydrocarbons
- transformations of alkyl halides and alcohols
- transformations of amines
- transformations of aldehydes and ketones
- transformations of carboxylic acids and related functional groups
- protecting groups for alcohols, amines, aldehydes, ketones and carboxylic acids

Part 2: Review and Expansion of Carbon-Carbon Bond Formation:

2.1 Reactions of Organometallic Compounds
- Grignard reagents (alkyl, alkenyl, alkynyl, aryl) + carbon electrophiles
- Organolithium reagents + carbon electrophiles
- Organocopper(I) reagents + carbon electrophiles

2.2 Stabilized Carbanions and Related Compounds
- carbanions from M-CH_2-M (M = -NO_2, -CO-R, -CO-OR, -C≡N, etc.)
- carbanions from M-CH_2-R
- Wittig reagents
- Acyl carbanions
- Aromatic nucleophiles (Electrophilic Aromatic Substitution)

2.3 Ring Closure and Ring Opening Reactions
- Intramolecular cyclization by nucleophile-electrophile interaction
- Pericyclic reactions

Part 3: Process Development
- Developing Process Flow Diagrams for batch processes
- Scale-based selection of synthetic routes, reagents, solvents and operating conditions
- Unit operations on lab/pilot/plant scales
- Work up procedures and safety hazards
- Product purification by extraction, crystallization, distillation, and chromatography
- Final product form and impurity considerations

Part 4: Retrosynthetic Analysis:
- disconnections, synthons, and reagents
- Strategies for linear target molecules
- 2-group disconnections (1,2-; 1,3-; 1,4-; and 1,5- patterns)
- Strategies for olefins and cyclic target molecules