Department of Chemistry Course Outline
SC/CHEM 4055 3.00 - Winter 2025
Enzyme Design in Virtual Reality

Course Description

This course introduces students to the fundamental principles and modern methods of enzyme design. Foundational topics of protein structure and the mechanisms of enzymatic activity are presented in the first part of the course. The students gain new appreciation of these concepts as they examine a variety of enzyme structures in Virtual Reality (VR). The second part of the course presents the theory and practice behind modern methods of rational enzyme design, directed evolution approaches and hybrid methods. The application of these concepts is then discussed using several examples of enzymes designed for bioremediation, natural product synthesis, and biofuel production. Throughout the course, the students' learning of the topics is supported and augmented by the use of VR technology as they examine, manipulate, design, and document various aspects of these molecules.

Prerequisites

SC/CHEM 3051 3.00, SC/BIOL 3051 3.00, or SC/BCHM 3051 3.00 (or permission of the instructor)

Course Instructor and Contact Information

Course Director:	Dr. Kyle Belozerov
	CB216 (Chemistry Building, Keele campus)
	vbelozer@yorku.ca
Student Hours:	By appointment

Schedule

Lectures: Tuesdays, 11:30 am – 2:30 pm, Curtis Lecture Hall 110 (CLH 110)

Please note that this course is delivered fully in-person, and most class activities and evaluations require the students to be physically present during class time. Therefore, arriving on time and attending class regularly are important.

Evaluation

In-class and Discord Participation	10%	Earned throughout the semester
Nanome Tips	5%	A one-page tip shared on Discord
Nano-quizzes	30%	Three quizzes, 10% each, will take place in the beginning of class on Feb 4, Mar 11, and Apr 1
Peer-reviewed Homework	20%	Four short group activities, 5% each, to be submitted as Nanome spatial recordings and reviewed by another group

Capstone Group Project	35%	The project will consist of the following components: • A 200–400-word proposal, including references, due on January 31 – **5%** • Group presentation of the project (date of your presentation will be scheduled during the first week of the semester) – **25%** • A 10-min spatial recording of the project, due on April 4 – **5%**

Additional details about evaluation components. Please read carefully!

1) In this course, students are expected to engage in active learning, both individually and in groups, during class time. Therefore, class attendance is required. Each student will earn "class participation" credit during each class by submitting a paper card at the end of the class. This credit will be based on engaging with the course material by asking and/or answering questions, providing comments, and working with peers. Up to two classes may be missed with no penalty, to accommodate for possible illnesses and other unforeseen circumstances. Therefore, a student would need to attend and participate in a minimum of 10 out of 12 classes to earn full participation credit. In-class participation may be supplemented by contributing to the course Discord server.

2) Nano-quizzes will be short (15-20 min), mostly or completely multiple-choice tests that will contain questions on the topics discussed in the previous 3-4 classes. Nano-quizzes will take place in the beginning of each class starting at 11:30 am. If a student misses a mini-quiz, a make-up quiz will be offered as arranged by the instructor. Nano-quizzes may involve group work and/or the use of the VR headset.

3) Homework questions will be posted on eClass and will require applying a concept learned in class to an enzyme structure from a database. Each group will collaborate to answer the question in the form of a short (5 min or so) spatial recording. Each group will upload their recording to eClass and email the file to their peer group for review. Thus, two groups will exchange their recordings, review them, and send back a brief (200-300 word) feedback on their work. Credit will be awarded based on completion of this peer-review activity. The constructive peer feedback should be used by each group to improve their subsequent homework submissions.

4) For the capstone project, students will form 4-member groups. Each group will select a particular class of enzymes that has been successfully engineered for an industrial application. Each group will conduct a thorough literature review on the advances made and future challenges associated with the selected class of enzymes and create and deliver a 20-25 min presentation during one of the last three classes of the semester. The presentation will include both a PowerPoint component (presented by 2 students) and live VR component (presented by the other 2 group members and projected onto the classroom screen). The instructor (and possibly a guest professor) will evaluate each presentation and award a grade based on the rubric (posted on

eClass). All presentations will be scheduled during the first week of classes (Jan 6 – Jan 10). In addition to the live presentation, each group will record a short VR spatial recording explaining the mechanism of their chosen enzyme and the structure-activity optimization for the industrial application. The spatial recording must be focused on showcasing the enzyme structure and utilizing as many advanced Nanome tools as needed for the effective presentation. The recordings will need to be uploaded to eClass by April 4, and will be reviewed and evaluated by the instructor.

Important Dates

Classes start:	January 6
Reading Week:	February 15 – 21
Drop Deadline:	March 14 (Last day to drop the course without receiving a grade)
Course withdrawal:	March 15 – April 4 (Course still appears on transcript as "W", but no grade is recorded)
End of classes:	April 4
Exams period:	April 10 – 26 **(**Please note there is no final exam in this course**)**

For additional important dates such as holidays, refer to the "Important Dates" *section of the Registrar's Website.*

Resources

1. eClass course site:
All lecture slides and other relevant material will be posted on eClass as the course proceeds. Announcements, grades, and other course information are communicated through the course eClass site.

2. No textbook is required for the course. All journal articles to be used in the course are freely available to registered students through the York University Library.

3. Each student will receive a Meta Quest 2 VR headset, two controllers, a charger, and a silicone face guard to take home and use for the duration of the semester. Students will be responsible for replacing AA batteries in the controllers as needed, and for the return of the above listed items in good working condition at the end of the semester.

4. Each student will be provided with an academic Nanome license free of charge, on a rolling basis (see posted schedule).

Learning Goals & Outcomes

Upon completion of the course, each student should be able to:

1) Explain the forces and interactions that underlie the formation of three-dimensional structures in enzyme molecules and be able to analyse structural models of enzymes in a Virtual Reality (VR) environment.

2) List the common mechanisms of enzymatic activity and relate these mechanisms to structural features of the active site and explain these features in VR.
3) List and explain the broad classes of approaches to designing novel enzyme functions and compare the advantages and disadvantages of the existing methods.
4) List and explain several specific examples of industrial applications of engineered enzymes and articulate why these applications benefit from designed enzymes as compared to traditional catalytic chemistry.
5) Discuss examples of enzymes that have been designed to perform novel functions and present the rationale for designed active site structure in the VR environment.

Course Content

The course will consist of three broad modules focused on the following topics:
(1) Protein structure and enzyme mechanisms;
(2) Modern approaches to designing enzymes with desired activities and characteristics;
(3) Application of enzyme design in bioremediation, synthesis of complex natural products and pharmaceuticals, and biofuel industry.
Each module will take up approximately one third of the course (4 weeks of instruction).

Experiential Education and E-Learning

- In-class group activities and discussions
- Learning to work in Virtual Reality environment using a cutting-edge molecular design software suite (Nanome Inc)
- Peer-review activities and group presentations
- Finding and analyzing primary scientific literature sources

Course Policies

1. E-MAIL ETIQUETTE:

- Use your Yorku email address as other email addresses (e.g., Hotmail) are filtered out by the university's email system and do not always reach their intended recipient. **Please do not use the Moodle email function or respond to course announcement emails.**
- I will try to respond within 2 business days, but this is not always possible. I typically do not check email between 5 pm and 9 am, nor on the weekends.
- **Subject line:** your name, student number and a brief indication of topic (*e.g.,* 'Question regarding gene regulation). I receive a lot of email and this practice helps me sort emails efficiently. **Emails without the required information will not receive a response.**
- **Please include your NAME at the end of each email.**
- I may not be able to offer individual tutoring by e-mail. **If your question requires me to type up several paragraphs to essentially repeat what was discussed in class, I may not be able to respond.** Please attend classes regularly and take careful notes during lectures. If you need extra help, please consider attending my office hours.

2. MISSED TESTS: Please see important notes under "Evaluation".

3. RE-MARKING REQUESTS:
- If you believe a written answer on a test was marked incorrectly you must submit a written rationale detailing the suspected error through eClass (instructions to be given at a later date) within 1 week of receiving a Crowdmark link to your marked paper. I will aim to address all re-marking requests within 1-2 weeks of receiving them.
- **NOTE: re-marking can result in the mark being raised, confirmed, or lowered.**
- To be fair and consistent with regards to the entire class, **individual grades are NOT negotiable**. We cannot provide 'extra credit' assignments. **Marks for assignments and tests are not 'rounded' or 'bell-curved'.** Contact me (vbelozer@yorku.ca) about marks **ONLY if there is a clear error in your mark (calculation, clerical, etc.) within ONE (1) week of the test score being made available to you.** It is highly unlikely that you will receive a response regarding any other mark-related queries.

4. YORK'S GRADING SCHEME

Letter	Point Value	Percentage	Definition
A+	9	90-100	Exceptional
A	8	80-89	Excellent
B+	7	75-79	Very Good
B	6	70-74	Good
C+	5	65-69	Competent
C	4	60-64	Fairly Competent
D+	3	55-59	Passing
D	2	50-54	Barely Passing
E	1	40-49	Marginally Failing
F	0	0-39	Failing

5. IMPORTANT COURSE INFORMATION FOR STUDENTS

All students are expected to familiarize themselves with the following information, available on the Senate Committee on Academic Standards, Curriculum & Pedagogy web page (see Reports, Initiatives, Documents) - http://www.yorku.ca/secretariat/senate/committees/ascp/index-ascp.html

- Ethics Review Process for research involving human participants:
  http://www.glendon.yorku.ca/research/obtain-ethics-approval/
- Accommodation for students with disabilities:
  http://www.glendon.yorku.ca/academic-services/exams/alternate-accommodation-for-tudents-with-disabilities/
- Student Rights and Responsibilities: http://oscr.students.yorku.ca/csrr
- Religious Observance Accommodation:
  http://www.glendon.yorku.ca/academic-services/exams/religious-accommodation/

- **6. ACADEMIC HONESTY:** Numerous students in Faculty of Science courses have been <u>charged with academic misconduct</u> when materials they uploaded to third party repository sites (e.g. Course Hero, One Class, etc.) were taken and used by unknown students in later offerings of the course. The Faculty's Committee on Examinations and Academic Standards (CEAS) found in these cases that the burden of proof in a charge of aiding and abetting had been met, since the uploading students had been found in all cases to be wilfully blind to the reasonable likelihood of supporting plagiarism in this manner. Accordingly, to avoid this risk, students are urged not to upload their work to these sites. **<u>Whenever a student submits work obtained through Course Hero or One Class, the submitting student will be charged with plagiarism and the uploading student will be charged with aiding and abetting.</u>** Note also that exams, tests, and other assignments are the copyrighted works of the professor assigning them, whether copyright is overtly claimed or not (i.e. whether the © is used or not). Scanning these documents constitutes copying, which is a breach of Canadian copyright law, and the breach is aggravated when scans are shared or uploaded to third party repository sites.

- **Course Policy on Generative Artificial Intelligence (AI tools)**

  Generative artificial intelligence (AI) tools have quickly become ubiquitous in internet research. In this course, we have no assignments that directly engage with AI and students are NOT REQUIRED to use AI tools for any of the course assignments. The use of AI tools is strictly prohibited in the use of exams. However, students are not restricted from using AI tools for assignments and discussion posts in this course so long as the following two conditions are met:

  1. While generative artificial intelligence (AI) – specifically, ChatGPT or Bing chatbot – can be used in the completion of written assignments and contributions to the online discussions, it will be used with the expectation that you use the AI tool to think with you, but not for you. AI tools are primarily developed for "natural language modelling" (speculating on how to put sentences together) and not for specialized research and analysis. Their knowledge base is derived from the indiscriminate scraping of random sites on the internet. None of the information provided is vetted or cited. Often AI tool produce erroneous or overly generalized knowledge, even though they are improving all the time. This means it is risky for students to use them in assignments. The AI tool may give you a place to start your research or point you in new directions, but usually they will not be sufficient to successfully complete an assignment. If you use another generative AI tool beyond ChatGPT and Bing, it will be considered an unauthorized use, and as a result, you will be violating the Senate Policy on Academic Honesty.

  2. The use of generative AI should be documented and cited. In the discussion forums, simply put in brackets after your answer "(this answer [or parts of this answer] were generated by ChatGPT [or Bing])". Credit the AI whenever you use the tool to generate text used in your assignment. Here is an example of how to cite in a footnote ChatGPT in the Chicago Style: · Text generated by ChatGPT, March 7, 2023, OpenAI, https://chat.openai.com/chat.

ChatGPT, response to "Explain how to make pizza dough from common household ingredients," March 7, 2023, OpenAI.

Use of generative AI outside these two conditions will constitute academic dishonesty under York University's Senate Policy on Academic Honesty. As a student in this course, it is your responsibility to understand when and how generative AI tools can be used to complete your assessments and activities. If you do not know whether an online resource or tool can be used in this course, please contact your instructor for guidance.

Note on evaluation for assignments using AI: When evaluating your work with generative AI, **I will be assessing the quality of your critical reflections and original contributions in accordance with York University's description of grades and grading schemes**.

- **RECORDING LECTURES:** Students are allowed to record lectures using their own voice recording devices. However, taking pictures or video recording of exam questions discussed in class will **NOT** be allowed. **Lecture recordings, slides, assignments and test questions are the intellectual property of the course instructor and CANNOT be uploaded or distributed to any third-party sites (see above section regarding ACADEMIC HONESTY. THIS STATEMENT APPLIES TO BOTH REMOTE & FACE-TO-FACE LECTURES.**

- **E-MAIL ETIQUETTE:** Use your Yorku email address as other email addresses (e.g., Hotmail, Gmail) are filtered out by the university's email system and do not always reach their intended recipient. **Please DO NOT use the Moodle email function or respond to course announcement emails.** I will try to respond within 1 business day, but this is not always possible. I typically do not check email between 6 pm and 9 am, nor on the weekends.

  Subject line: your name, student number and a brief indication of topic (*e.g.,* 'Question regarding genetics). **Emails without the required information will not receive a response. Please include your NAME at the end of each email.** I will not be able to offer individual tutoring by email. **If your question requires me to type up several paragraphs to essentially repeat what was posted, I may not be able to respond.** Please attend class, listen to the lecture recordings and take good notes.

7. FAMILY-FRIENDLY ENVIRONMENT IN THE CLASSROOM:
- For older children and babies, I understand that minor illnesses and unforeseen disruptions in childcare often put parents in the position of having to choose between missing class to stay home with a child and leaving him or her with someone you or the child does not feel comfortable with. While this is not meant to be a long-term childcare solution, occasionally bringing a child to class in order to cover gaps in care is perfectly acceptable.
- I ask that all students work with me to create a welcoming environment that is respectful of all forms of diversity, including diversity in parenting status.
- In all cases where babies and children come to class, I ask that you sit close to the door so that if your little one needs special attention and is disrupting learning for other students, you may step outside until their need has been met. Non-parents in the class, please reserve seats near the door for your parenting classmates.

- Finally, I understand that often the largest barrier to completing your coursework once you become a parent is the tiredness many parents feel in the evening once children have finally gone to sleep. The struggles of balancing school, childcare and often another job are exhausting! I hope that you will feel comfortable disclosing your student-parent status to me. This is the first step in my being able to accommodate any special needs that arise. While I maintain the same high expectations for all student in my classes regardless of parenting status, I am happy to problem solve with you in a way that makes you feel supported as you strive for school-parenting balance. Thank you for the diversity you bring to our classroom!

University Policies

ACADEMIC HONESTY & INTEGRITY

York students are required to maintain the highest standards of academic honesty and they are subject to the Senate Policy on Academic Honesty https://www.yorku.ca/secretariat/policies/policies/academic-conduct-policy-and-procedures/. The Policy affirms the responsibility of faculty members to foster acceptable standards of academic conduct and of the student to abide by such standards.

There is also an academic integrity website with comprehensive information about academic honesty and how to find resources at York to help improve students' research and writing skills, and cope with University life. Students are expected to review the materials on the Academic Integrity website at https://spark.library.yorku.ca/academic-integrity-what-is-academic-integrity/

Artificial Intelligence (AI) Apps

According to York's Senate Policy on Academic Honesty, using AI apps such as such as ChatGPT, GPT-3, DALL-E, among others to complete academic work without your instructor's knowledge or permission, is considered to be a breach of academic honesty. More specifically, using text-generating tools (such as ChatGPT) would be considered to be cheating (Senate Policy, section 2.1.1) and using imagegenerating tools (such as DALL-E) would be considered to be plagiarism (Senate Policy, section 2.1.3). You may find that certain instructors will allow the use of these tools for certain assessments, yet others will not allow their use. If you're not sure whether using an AI app for your academic work is acceptable, it is recommended that you:

· Carefully review the guidelines for your assessments

· Check for any messages from your instructor on eClass

· Ask your instructor or TA if they are permitting the use of these tools

Additionally, you are encouraged to keep all of your research notes and draft versions of your work. You may be asked to present these if it is suspected that an AI app was used to help complete your work. These drafts can be used to show how this work developed, and to provide evidence that the work is your own.

Group Messaging Tools

Group messaging platforms, such as Discord or WhatsApp, can be helpful tools that connect students and support learning. However, such tools can lead to academic honesty violations when students share or use answers to homework tasks, quizzes, tests, or exams, or when students collaborate on individual assignments. According to York's Senate Policy on Academic Honesty these behaviours may lead to a penalty. Moderators of these groups are required to clearly communicate the group's purpose and to remind students of the expectations for academic honesty. Being a member of such a group is not a breach of academic honesty or any other university policy. However, if you witness academically dishonest behaviour, it is strongly recommended that you leave the group. If you are unsure whether the behaviour is a violation of academic honesty, check with your TA or instructor. For detailed information about expectations for academic honesty, please refer to York's Senate Policy

on Academic Honesty.

Homework Help Sites

According to homework sites (such as Chegg), their services are intended to support students' understanding of course material. Despite this, cheating occurs on tests and exams when students post their test or exam questions to these sites during the assessment in order to obtain answers from one of their experts. Using the answers provided is a breach of academic honesty, according to York's Senate Policy on Academic Honesty. If you're struggling with course material, understanding expectations, or in any other way, reach out to your instructor or TA instead of relying on homework help sites to acquire assessment answers. For authorized resources and sources of help at York, please visit: https://www.yorku.ca/unit/vpacad/academic-integrity/student-resources/.

Contract Cheating

Contract cheating occurs when a third party completes a student's work, and the student then submits that work as their own. Third parties can include: freelance academic writers or tutors, online essay writing companies, friends, classmates, or even family members. Contract cheating is considered to be a serious type of academic dishonesty that carries severe penalties. Besides penalties imposed by the university, contracting a third party to complete academic work carries the additional risks of identity theft and blackmail. If you are unsure whether a certain resource is a legitimate source of help, check with your TA or instructor. For authorized resources and sources of help at York, please visit: https://www.yorku.ca/unit/vpacad/academic-integrity/student-resources/. As well, for detailed information about expectations for academic honesty, please refer to York's Senate Policy on Academic Honesty.

Unauthorized Collaboration

Unauthorized collaboration occurs when students work together on assessments without their instructor's permission. This can include working together to solve homework problems, comparing their homework, test or exam answers, collaborating to complete assignments, or

having someone else write or revise an assignment. Sometimes collaborating on assessments with other students is acceptable, yet at other times, individual effort is required. This can vary by course, instructor, or assessment. Even when it comes to group assignments, individual work may be required at different stages. If you are unsure whether collaborating on assigned work is permitted or the extent of collaboration that is acceptable, review the instructions for that assessment, and/or ask your instructor or TA. Note: even if collaboration on an assessment is permitted, it is never acceptable copy someone else's work or allow them to copy yours.

Plagiarism

Plagiarism is defined as misusing another person's published or unpublished work by presenting their ideas, writing or other intellectual property as one's own without proper acknowledgement (Senate Policy on Academic Honesty, section 2.1.3.). There are a number of acts that are considered to be plagiarism, for example:

- copying content word-for-word from a source without proper citation;
- paraphrasing from a source without proper citation; submitting work you have already submitted for another course without the instructor's approval;
- rewording someone else's work which you submit as your own;
- having a third party complete work in whole then submitting it as one's own (also known as contract cheating).

Although plagiarism is often thought to involve words and ideas, it can also involve drawings, paintings, photographs, programming code, statistics, presentations, musical scores, among other types of content. Even if the act of plagiarism was unintentional, you can still receive a penalty. To avoid plagiarism, keep good track of any outside sources you use, and ensure that you cite sources properly. For more help on how to avoid plagiarism, contact the Library, Writing Centre, or your instructor or TA.

Access/Disability

York University is committed to principles of respect, inclusion and equality of all persons with disabilities across campus. The University provides services for students with disabilities (including physical, medical, learning and psychiatric disabilities) needing accommodation related to teaching and evaluation methods/materials. These services are made available to students in all Faculties and programs at York University.

Students in need of these services are asked to register with disability services as early as possible to ensure that appropriate academic accommodation can be provided with advance notice. You are encouraged to schedule a time early in the term to meet with each professor to discuss your accommodation needs. Please note that registering with disabilities services and discussing your needs with your professors is necessary to avoid any impediment to receiving the necessary academic accommodations to meet your needs.

Additional information is available at the following websites:
    Counselling & Disability Services at Glendon

https://www.glendon.yorku.ca/counselling/disability/

Accessibility services at Glendon https://www.yorku.ca/glendon/supports-and-services/glendon-   accessibility-services/

Counselling & Disability Services https://accessibility.students.yorku.ca/

York Accessibility Hub https://accessibilityhub.info.yorku.ca/

*Please note that it is the student's responsibility to Register with Glendon Accessibility Services https://www.yorku.ca/glendon/current-students/alternate-exams/ AND to arrange an appointment with the Alternate Test/Exam Scheduling center THREE WEEKS prior to the test/exam date.

Ethics Review Process

York students are subject to the York University *Policy for the Ethics Review Process for Research Involving Human Participants.* In particular, students proposing to undertake research involving human participants (e.g., interviewing the director of a company or government agency, having students complete a questionnaire, etc.) are required to submit an *Application for Ethical Approval of Research Involving Human Participants* at least one month before you plan to begin the research. If you are in doubt as to whether this requirement applies to you, contact your Course Director immediately.

Religious Observance Accommodation

York University is committed to respecting the religious beliefs and practices of all members of the community, and making accommodations for observances of special significance to adherents https://registrar.yorku.ca/enrol/dates/religious-accommodation-resource-2023-2024

Should any of the dates specified in this syllabus for an in-class test or examination pose such a conflict for you, contact the Course Director within the first three weeks of class. Similarly, should an assignment to be completed in a lab, practicum placement, workshop, etc., scheduled later in the term pose such a conflict, contact the Course director immediately. Please note that to arrange an alternative date or time for an examination scheduled in the formal examination periods (December and April/May), students must complete an Examination Accommodation Form, which can be obtained from Student Client Services, Student Services Centre or online at https://secure.students.yorku.ca/pdf/religious-accommodation-agreement-final-examinations.pdf

Student Conduct in Academic Situations

Students and instructors are expected to maintain a professional relationship characterized by courtesy and mutual respect. Moreover, it is the responsibility of the instructor to maintain an appropriate academic atmosphere in the classroom and other academic settings, and the responsibility of the student to cooperate in that endeavour. Further, the instructor is the best person to decide, in the first instance, whether such an atmosphere is present in the class. The policy and procedures governing disruptive and/or harassing behaviour by students in academic situations is available at - http://secretariat-

policies.info.yorku.ca/policies/disruptive-andor-harassing-behaviour-in-academic-situations-senate-policy/

Hyflex classrooms

Hyflex sessions are digitally transmitted and may be recorded to support teaching and learning in the classroom. As a result, York University may collect your image, voice,name, personal views and opinions, and course work under the authority of The York University Act, 1965, and for use in related educational purposes. Students who participate in a Hyflex session are consenting to have their video or image transmitted and/or recorded. If you have concerns with such transmission or recording, sit in the designated seating area which is outside of the camera range. In addition, students who participate orally are consenting to have their voices, personal views and opinions transmitted and/or recorded. If you do not consent to the transmission or recording of your voice, please use the text-based chat function communicate during class. Students are not permitted to use any third-party software or application to record a transmitted Hyflex session. If you have any questions about the collection or use of your personal information, please contact your instructor or the Privacy Office at info.privacy@yorku.ca.