



COURSE OUTLINE

1. **Course:** BCEM 577, Biomolecular Simulation - Fall 2022

Lecture 01 : TR 11:00 - 12:15 in ST 059

Instructor	Email	Phone	Office	Hours
Dr Peter Tieleman	tieleman@ucalgary.ca	403 220-2966	BI 489	By email appointment

To account for any necessary transition to remote learning for the current semester, courses with in-person lectures, labs, or tutorials may be shifted to remote delivery for a certain period of time. In addition, adjustments may be made to the modality and format of assessments and deadlines, as well as to other course components and/or requirements, so that all coursework tasks are in line with the necessary and evolving health precautions for all involved (students and staff).

In Person Delivery Details:

Lecture 01: TR 11:00-12:15 in ST 059

Lab 1 (B01): M 16:00 - 19:50 in BI 190

Lab 2 (B02): W 16:00 - 19:50 in BI 190

Lectures and labs will be delivered in person

Re-Entry Protocol for Labs and Classrooms:

To limit the spread of COVID-19 on campus, the University of Calgary has implemented safety measures to ensure the campus is a safe and welcoming space for students, faculty and staff. The most current safety information for campus can be found [here](#).

Course Site:

D2L: BCEM 577 L01-(Fall 2022)-Biomolecular Simulation

Note: Students must use their U of C account for all course correspondence.

Equity Diversity & Inclusion:

The University of Calgary is committed to creating an equitable, diverse and inclusive campus, and condemns harm and discrimination of any form. We value all persons regardless of their race, gender, ethnicity, age, LGBTQIA2S+ identity and expression, disability, religion, spirituality, and socioeconomic status. The Faculty of Science strives to extend these values in every aspect of our courses, research, and teachings to better promote academic excellence and foster belonging for all.

The Biological Sciences Equity Committee acknowledges there are persistent barriers that prevent such accessibility and hinder our progress towards EDI. Our representatives (faculty, staff, postdocs, graduate and undergraduate students) are committed to addressing any concerns and work towards proactive solutions that enact necessary change within the department. To submit anonymous questions, comments or concerns regarding EDI related issues, please reach out to our Chair, Constance Finney (constance.finney@ucalgary.ca), or a committee representative of your choice at <https://science.ucalgary.ca/biological-sciences/about/equity-diversity-and-inclusion>

2. **Requisites:**

See section [3.5.C](#) in the Faculty of Science section of the online Calendar.

Prerequisite(s):

Biochemistry 341 or 393; and Biochemistry 471 or Chemistry 371.

3. **Grading:**

The University policy on grading and related matters is described in [F.1](#) and [F.2](#) of the online University Calendar.

In determining the overall grade in the course the following weights will be used:

Course Component	Weight	Due Date (duration for exams)	Modality for exams	Location for exams
Midterm 1	30%	Oct 18 2022 at 11:00 am (75 Minutes)	in-person	In class
Lab 2 ¹	14%	Oct 19 2022		
Lab 3 ²	13%	Nov 30 2022		
Lab 4 ³	13%	Dec 14 2022		
Registrar Scheduled Final Exam	30%	Will be available when the final exam schedule is released by the Registrar	in person	Will be available when the final exam schedule is released by the Registrar

¹ Lab report is due 2 weeks after the last lab session for lab 2. The due date will be different depending on which group you are in. For the Monday group, the due date is Oct. 17. For the Wednesday group, the due date is Oct. 19.

² Lab report is due 2 weeks after the last lab session for lab 3. The due date will be different depending on which group you are in. For the Monday group, the due date is Nov. 28. For the Wednesday group, the due date is Nov. 30.

³ Lab report is due 2 weeks after the last lab session for lab 4. The due date will be different depending on which group you are in. For the Monday group, the due date is Dec. 12. For the Wednesday group, the due date is Dec. 14.

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows.

	A+	A	A-	B+	B	B-	C+	C	C-	D+	D
Minimum % Required	95 %	85 %	82 %	79%	76%	72 %	68 %	64%	60%	55 %	50 %

This course will have a Registrar Scheduled Final exam that will be delivered in-person and on campus. [The Final Examination Schedule](#) will be published by the Registrar's Office approximately one month after the start of the term. The final exam for this course will be designed to be completed within 2 hours.

Lab 1 is required to learn how to use the software environment but has no assessed components.

The University of Calgary offers a [flexible grade option](#), Credit Granted (CG) to support student's breadth of learning and student wellness. Faculty units may have additional requirements or restrictions for the use of the CG grade at the faculty, degree or program level. To see the full list of Faculty of Science courses where CG is not eligible, please visit the following website: <https://science.ucalgary.ca/current-students/undergraduate/program-advising/flexible-grading-option-cg-grade>

4. Missed Components Of Term Work:

The university has suspended the requirement for students to provide evidence for absences. Please do not attend medical clinics for medical notes or Commissioners for Oaths for statutory declarations.

In the event that a student legitimately fails to submit any online assessment on time (e.g. due to illness etc...), please contact the course coordinator, or the course instructor if this course does not have a coordinator to arrange for a re-adjustment of a submission date. Absences not reported within 48 hours will not be accommodated. If an excused absence is approved, one possible arrangement is that the percentage weight of the legitimately missed assignment could also be pro-rated among the components of the course. This option is at the discretion of the coordinator and may not be a viable option based on the design of this course.

5. Scheduled Out-of-Class Activities:

There are no scheduled out of class activities for this course.

6. Course Materials:

Recommended Textbook(s):

Ivet Bahar, Robert L. Jernigan, Ken Dill, *Protein Actions: Principles and Modeling*: Garland Science.

Lecture notes, journal articles, and downloadable materials highlighted in the lectures. Textbook is not essential but probably the best textbook-level explanation of simulation and modeling background and applications to proteins.

In order to successfully engage in their learning experiences at the University of Calgary, students taking online, remote and blended courses are required to have reliable access to the following technology:

- A computer with a supported operating system, as well as the latest security, and malware updates;
- A current and updated web browser;
- Webcam/Camera (built-in or external);
- Microphone and speaker (built-in or external), or headset with microphone;
- Current antivirus and/or firewall software enabled;
- Stable internet connection.

For more information please refer to the UofC [ELearning](#) online website.

7. Examination Policy:

A calculator is required on tests/exams. No other materials are allowed (closed book).

Students should also read the Calendar, [Section G](#), on Examinations.

8. Approved Mandatory And Optional Course Supplemental Fees:

There are no mandatory or optional course supplemental fees for this course.

9. Writing Across The Curriculum Statement:

For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) can be a factor in the evaluation of the work. See also [Section E.2](#) of the University Calendar.

10. Human & Living Organism Studies Statements:

Students will not participate as subjects or researchers in human studies.

See also [Section E.5](#) of the University Calendar.

STUDIES IN THE BIOLOGICAL SCIENCES INVOLVE THE USE OF LIVING AND DEAD ORGANISMS. Students taking laboratory and field-based courses in these disciplines can expect involvement with and experimentation on such materials. Students perform dissections on dead or preserved organisms in some courses. In particular courses, students experiment on living organisms, their tissues, cells, or molecules. Sometimes field work requires students to collect a variety of living materials by many methods, including humane trapping.

All work on humans and other animals conforms to the Helsinki Declaration and to the regulations of the Canadian Council on Animal Care. The Department strives for the highest ethical standards consistent with stewardship of the environment for organisms whose use is not governed by statutory authority. Individuals contemplating taking courses or majoring in one of the fields of study offered by the Department of Biological Sciences should ensure that they have fully considered these issues before enrolling. Students are advised to discuss any concern they might have with the Undergraduate Program Director of the Department.

Students are expected to be familiar with [Section SC.4.1](#) of the University Calendar.

11. Reappraisal Of Grades:

A student wishing a reappraisal, should first attempt to review the graded work with the Course coordinator/instructor or department offering the course. Students with sufficient academic grounds may request a reappraisal. Non-academic grounds are not relevant for grade reappraisals. Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See [Section I.3](#) of the University Calendar.

- Term Work:** The student should present their rationale as effectively and as fully as possible to the Course coordinator/instructor within **ten business days** of either being notified about the mark, or of the item's return to the class. If the student is not satisfied with the outcome, the student shall submit the Reappraisal of Graded Term work [form](#) to the department in which the course is offered within 2 business days of receiving the decision from the instructor. The Department will arrange for a reappraisal of the work within

the next ten business days. The reappraisal will only be considered if the student provides a detailed rationale that outlines where and for what reason an error is suspected. See sections [I.1](#) and [I.2](#) of the University Calendar

- b. **Final Exam:** The student shall submit the request to Enrolment Services. See [Section I.3](#) of the University Calendar.

12. Other Important Information For Students:

- a. **Mental Health** The University of Calgary recognizes the pivotal role that student mental health plays in physical health, social connectedness and academic success, and aspires to create a caring and supportive campus community where individuals can freely talk about mental health and receive supports when needed. We encourage you to explore the mental health resources available throughout the university community, such as counselling, self-help resources, peer support or skills-building available through the SU Wellness Centre (Room 370, MacEwan Student Centre, [Mental Health Services Website](#)) and the Campus Mental Health Strategy website ([Mental Health](#)).
- b. **SU Wellness Services:** For more information, see their [website](#) or call [403-210-9355](#).
- c. **Sexual Violence:** The Sexual Violence Support Advocate, Carla Bertsch, can provide confidential support and information regarding sexual violence to all members of the university community. Carla can be reached by email (svsa@ucalgary.ca) or phone at [403-220-2208](#). The complete University of Calgary policy on sexual violence can be viewed [here](#).
- d. **Misconduct:** Academic integrity is the foundation of the development and acquisition of knowledge and is based on values of honesty, trust, responsibility, and respect. We expect members of our community to act with integrity. Research integrity, ethics, and principles of conduct are key to academic integrity. Members of our campus community are required to abide by our institutional [Code of Conduct](#) and promote academic integrity in upholding the University of Calgary's reputation of excellence. Some examples of academic misconduct include but are not limited to: posting course material to online platforms or file sharing without the course instructor's consent; submitting or presenting work as if it were the student's own work; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; borrowing experimental values from others without the instructor's approval; falsification/fabrication of experimental values in a report. Please read the following to inform yourself more on academic integrity:

[Student Handbook on Academic Integrity](#)
[Student Academic Misconduct Policy](#) and [Procedure](#)
[Faculty of Science Academic Misconduct Process](#)
[Research Integrity Policy](#)

Additional information is available on the [Student Success Centre Academic Integrity page](#)

- e. **Academic Accommodation Policy:**

It is the student's responsibility to request academic accommodations according to the University policies and procedures listed below. The student accommodation policy can be found at: <https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Student-Accommodation-Policy.pdf>

Students needing an accommodation because of a disability or medical condition should communicate this need to Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities: <https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Accommodation-for-Students-with-Disabilities-Procedure.pdf>.

Students needing an accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, by filling out the [Request for Academic Accommodation Form](#) and sending it to Lisa Gieg by email imgieg@ucalgary.ca preferably 10 business days before the due date of an assessment or scheduled absence.

- f. **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). Students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page. For more information, see [Legal Services](#) website.

- g. **Student Union Information:** [SU contact](#), Email SU Science Rep: sciencerep1@su.ucalgary.ca, [Student Ombudsman](#)

- h. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction ([USRI](#)) survey and the Faculty of Science Teaching Feedback form provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses. Your responses make a difference - please participate in these surveys.
- i. **Copyright of Course Materials:** All course materials (including those posted on the course D2L site, a course website, or used in any teaching activity such as (but not limited to) examinations, quizzes, assignments, laboratory manuals, lecture slides or lecture materials and other course notes) are protected by law. These materials are for the sole use of students registered in this course and must not be redistributed. Sharing these materials with anyone else would be a breach of the terms and conditions governing student access to D2L, as well as a violation of the copyright in these materials, and may be pursued as a case of student academic or [non-academic misconduct](#), in addition to any other remedies available at law.

Course Outcomes:

- Explain the concept of a hierarchy of physical models to mathematically describe biochemical systems
- Explain and apply the concept of energy functions and landscapes in molecular simulation and docking
- Explain and use the connection between probabilities and free energies to link simulations and experiments
- Explain the main principles behind molecular dynamics simulation
- Use knowledge of 1-4 in setting up, running, and analyzing a simple molecular dynamics simulation
- Explain the main steps, approximations, and limitations in homology modeling of protein structures and docking small molecules to proteins
- Use knowledge of 6 in practical work to make an homology model of a protein and dock small molecules
- Critically read research articles that use molecular simulation techniques, interpret figures/tables from such articles, broadly understand the methods used, and have some idea of the limitations and validity of the results
- Work effectively as part of a team in labs and literature presentations and provide constructive feedback to team members
- Communicate effectively both in writing and orally

Electronically Approved - Sep 02 2022 17:52

Department Approval