



UNIVERSITY OF CALGARY  
FACULTY OF SCIENCE  
DEPARTMENT OF BIOLOGICAL SCIENCES  
COURSE OUTLINE

1. **Course: BIOCHEMISTRY 577 – BIOMOLECULAR SIMULATION**

Lecture Sections: L01 TR 9:30-10:45 ST 125 WINTER 2018

Lab Section: B01 W 2:00-5:50 BI 182

**Course Coordinator/**

**Instructor:** Dr. P. Tieleman BI 415 220-2966 tieleman@ucalgary.ca

Course website or Desire 2 Learn (D2L) course name: BCEM 577

Biological Sciences Department BI 186; (403) 220-3140; biosci@ucalgary.ca

2. **PREREQUISITE(S):** One of Biochemistry 341 or 393 and one of Biochemistry 471 or Chemistry 371

See section 3.5.C in the Faculty of Science section of the online Calendar

(<http://www.ucalgary.ca/pubs/calendar/current/sc-3-5.html>)

3. **Grading:** The University policy on grading and related matters is described in sections F.1 and F.2 of the online University Calendar. In determining the overall grade in the course the following weights will be used:

Midterm Exam/ Assignment	30%	In Class	Feb. 13, 2018
Lab Assignments	40%		
Final Exam	30%		

There will be a final examination scheduled by the Registrar.

Letter Grade	A+	A	A-	B+	B	B-	C+	C	C-	D+	D
Min. Percent Required	95	86	82	78	74	70	66	62	58	54	50

Each piece of work (presentations, assignment, midterm test or final examination) submitted by the student will be assigned a percentage score. The student's average percentage score for the various components 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.

4. **Missed Components of Term Work:** The regulations of the Faculty of Science pertaining to this matter are found in the Faculty of Science area of the Calendar in Section 3.6. It is the student's responsibility to familiarize himself/herself with these regulations. See also Section E.6 of the University Calendar

5. **Scheduled out-of-class activities:** Dates and times of approved class activities held outside of class hours. N/A

REGULARLY SCHEDULED CLASSES HAVE PRECEDENCE OVER ANY OUT-OF-CLASS-TIME-ACTIVITY.

6. **Course Materials:** Textbook: Protein Actions: Principles and Modeling, Bahar, Jernigan and Dill, Garland Science 2017

7. **Examination Policy:** Exams are open book. Students should also read the Calendar, Section G, on Examinations.

8. **Writing across the curriculum statement:** In this course, the quality of the student's writing in the assignment will be a factor in its evaluation. See also Section E.2 of the University Calendar.

9. **OTHER IMPORTANT INFORMATION FOR STUDENTS:**

- (a) **Misconduct:** Academic misconduct (cheating, plagiarism, or any other form) is a very serious offence that will be dealt with rigorously in all cases. A single offence may lead to disciplinary probation or suspension or expulsion. The Faculty of Science follows a zero tolerance policy regarding dishonesty. Please read the sections of the University Calendar under [Section K. Student Misconduct](#) to inform yourself of definitions, processes and penalties.
- (b) **Assembly Points:** In case of emergency during class time, be sure to FAMILIARIZE YOURSELF with the information on [assembly points](#).
- (c) **Student Accommodations:** Students needing an Accommodation because of a Disability or medical condition should contact Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities available at [http://www.ucalgary.ca/policies/files/policies/procedure-for-accommodations-for-students-with-disabilities\\_0.pdf](http://www.ucalgary.ca/policies/files/policies/procedure-for-accommodations-for-students-with-disabilities_0.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, preferably in writing, to the Associate Head of Biological Sciences, Dr. H. Addy by email [addy@ucalgary.ca](mailto:addy@ucalgary.ca) or phone 403 220-3140.
- (d) **Safewalk:** Campus Security will escort individuals day or night (<http://www.ucalgary.ca/security/safewalk/>). Call 220-5333 for assistance. Use any campus phone, emergency phone or the yellow phones located at most parking lot pay booths.
- (e) **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPPA). As one consequence, 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 also <http://www.ucalgary.ca/secretariat/privacy>.
- (f) **Student Union Information:** VP Academic Phone: 403 220-3911 Email: [suvpaca@ucalgary.ca](mailto:suvpaca@ucalgary.ca)  
SU Faculty Rep. Phone: 403 220-3913 Email: [science1@su.ucalgary.ca](mailto:science1@su.ucalgary.ca), [science2@su.ucalgary.ca](mailto:science2@su.ucalgary.ca) and [science3@su.ucalgary.ca](mailto:science3@su.ucalgary.ca);  
Student Ombuds Office: 403 220-6420 Email: [ombuds@ucalgary.ca](mailto:ombuds@ucalgary.ca); <http://ucalgary.ca/provost/students/ombuds>
- (g) **Internet and Electronic Device Information:** You can assume that in all classes that you attend, your cell phone should be turned off unless instructed otherwise. Also, communication with other individuals, via laptop computers, Blackberries or other devices connectable to the Internet is not allowed in class time unless specifically permitted by the instructor. If you violate this policy you may be asked to leave the classroom. Repeated abuse may result in a charge of misconduct.
- (h) **U.S.R.I.:** At the University of Calgary, feedback provided by students through the Universal Student Ratings of Instruction (USRI) survey provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses ([www.ucalgary.ca/usri](http://www.ucalgary.ca/usri)). Your responses make a difference - please participate in USRI Surveys.

Department Approval \_\_\_\_\_ ORIGINAL SIGNED \_\_\_\_\_ Date \_\_\_\_\_

## **Learning outcomes**

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

1. explain the concept of a hierarchy of physical models to mathematically describe biochemical systems
2. explain and apply the concept of energy functions and landscapes in molecular simulation and docking
3. explain and use the connection between probabilities and free energies to link simulations and experiments
4. explain the main principles behind molecular dynamics simulation
5. use knowledge of 1-4 in setting up, running, and analyzing a simple molecular dynamics simulation
6. explain the main steps, approximations, and limitations in homology modeling of protein structures and docking small molecules to proteins
7. use knowledge of 6 in practical work to make an homology model of a protein and dock small molecules
8. 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
9. work effectively as part of a team in labs and provide constructive feedback to team members
10. communicate effectively in writing

## Tentative schedule:

### January

Lecture 1	1/9/2018	Introduction: models and simulations, learning objectives
Lecture 2	1/11/2018	Hierarchy of models, approximations
Lecture 3	1/16/2018	Protein structure/physics
LAB 1	1/17/2018	Linux/VMD intro
Lecture 4	1/18/2018	Membrane structure, nucleic acids
Lecture 5	1/23/2018	Elastic networks
Lecture 6	1/25/2018	Entropy and sampling
Lecture 7	1/30/2018	Molecular dynamics

### February

Lecture 8	2/1/2018	Molecular dynamics
Lecture 9	2/6/2018	Coarse graining
LAB 2	2/7/2018	MD lab
Lecture 10	2/8/2018	Examples
<b>Lecture 11</b>	<b>2/13/2018</b>	<b>Midterm</b>
LAB 2	2/14/2018	MD lab
Lecture 12	3/1/2018	Electrostatics

### March

Lecture 13	3/6/2018	Homology modeling 1
LAB 3	3/7/2018	Homology modeling
Lecture 14	3/8/2018	Homology modeling 2
LAB 3	3/14/2018	Homology modeling
Lecture 15	3/15/2018	Drug design 1
Lecture 16	3/20/2018	Drug design 2
LAB 4	3/21/2018	Docking
Lecture 17	3/22/2018	examples
LAB 4	3/28/2018	Docking
Lecture 18	3/29/2018	CAVE (Virtual reality environment)

### April

Lecture 19	4/10/2018	Questions
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