



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

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

Lecture Sections: L01 TR 09:30-10:45 ST 059 WINTER 2016
Instructor: Dr. D.P. Tieleman BI 415 220-2966 tieleman@ucalgary.ca
D2L course name: W2016BCEM577L01

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 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:

Lab Component	30%
Midterm I	35 %
Final Exam	35 %

There will be a final exam scheduled by the Registrar's Office.

Each piece of work (laboratory report, 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.3](#) of the University Calendar

Midterm Exam February 25, 2016 In-class

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

For late submissions of lab reports, there will be a 10% penalty for the first day, 25% for the second day, 50% for the third day, and 100% after that.

5. **Course Materials:**

TEXT: Recommended: Andrew Leach – Molecular Modelling: principles and applications. Prentice Hall, 2001. Don't buy this book, the library has several copies and the book is not required. Exams are based on lecture notes.

6. **Examination Policy:** Students are required to have standard non-programmable calculators. Exams are closed-book. Students should also read the Calendar, [Section G](#), on Examinations.

7. **Writing across the curriculum statement:** e.g. "In this course, the quality of the student's writing in laboratory reports will be a factor in the evaluation of those reports." See also [Section E.2](#) of the University Calendar.

8. 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.

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 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 (FOIPP). 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
SU Faculty Rep. Phone: 403 220-3913 Email: science1@su.ucalgary.ca, science2@su.ucalgary.ca and science3@su.ucalgary.ca;
Student Ombuds Office: 403 220-6420 Email: 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). Your responses make a difference - please participate in USRI Surveys.

Department Approval _____ ORIGINAL SIGNED _____ Date _____

UNIVERSITY OF CALGARY
DEPARTMENT OF BIOLOGICAL SCIENCES

BIOCHEMISTRY 577
BIOMOLECULAR SIMULATION

TERM: Winter 2016 SECTION NO: 01

A student may not register in a course unless they have a grade of at least C- in each prerequisite course.

COURSE COORDINATOR: **Dr. P.T. Tieleman** BI 415 220-2966 tieleman@ucalgary.ca

LECTURERS: Dr. P.T. Tieleman BI 415 220-2966 tieleman@ucalgary.ca
Dr. V. Corradi BI 490 220-6873 vcorradi@ucalgary.ca

LECTURES: TR 09:30-10:45 ST 059

TUTORIAL/LAB: T 14:00-17:50 BI 190

TEXT: Recommended: Recommended Readings will be posted on D2L along with lectures.

RESERVE READING ROOM: See page on D2L.

MARK DISTRIBUTION: A. Composition of Final Grade

Lab Component	30%
Midterm I	35 %
Final Exam	35 %

GRADING SCALE

86 A
82 A-
78 B+
74 B
70 B-
66 C+
62 C
58 C-
54 D+
50 D
<50 F

BCEM 577 – Biomolecular Simulation

Winter 2016 TENTATIVE LECTURE SCHEDULE

Lectures are Tuesday and Thursday, 9:30 - 10:45

Labs are Tuesday 14:00 - 17:50

Lecture 1	1/12/2016	Introduction: models and simulations, learning objectives
Lecture 2	1/14/2016	Hierarchy of models, approximations
Lecture 3	1/19/2016	Physics background
LAB 1	1/19/2016	Linux/VMD intro
Lecture 4	1/21/2016	Physics background
Lecture 5	1/26/2016	Physics background
Lecture 6	1/28/2016	Physics background
Lecture 7	2/2/2016	Molecular dynamics 1
February		
Lecture 8	2/4/2016	Molecular dynamics 2
Lecture 9	2/9/2016	Free energy
LAB 2	2/9/2016	MD lab
Lecture 10	2/11/2016	Molecular dynamics applications
Reading week	14-21 February	
Lecture 11	2/23/2016	Tutorial
LAB 2	2/23/2016	MD lab
Lecture 12	2/25/2016	Midterm
Lecture 13	3/1/2016	Electrostatics
March		
Lecture 14	3/3/2016	Electrostatics
Lecture 15	3/8/2015	Homology modeling 1
LAB 3	3/8/2016	Homology modeling lab
Lecture 16	3/10/2016	Homology modeling 2
Lecture 17	3/15/2016	CASP/CAPRI
LAB 3	3/15/2016	Homology modeling lab
Lecture 18	3/17/2016	Drug design 1
Lecture 19	3/22/2016	Drug design 2
LAB 4	3/22/2016	Docking lab
Lecture 20	3/24/2016	Examples
Lecture 21	3/29/2016	Coarse-graining
LAB 4	3/29/2016	Docking lab

April		
Lecture 22	3/31/2016	3D CAVE
Lecture 23	4/5/2016	Examples
Lecture 24	4/7/2016	Examples; Warshel visiting (Nobel prize Chemistry)
Lecture 25	4/12/2016	Examples/questions