BIOL/BCBP 4550/6420, Molecular Modeling. SPRING 2021

This course covers the theory and practice of molecular modeling, including homology-based modeling of proteins, energy minimization, molecular dynamics, structure-based alignment, protein design, and docking.

Place: remote **Time**: 8-9:50 T,F **Office hours**: F 10-12.

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Web sites: RPI LMS.

REQUIRED TEXT: None. *Required readings will be posted on the website.*

SOFTWARE: MOE (Available on institute-maintained computers in the classroom and VCC.)

GRADING: Homework 35%‡ Midterm exam 25%• Term project 15%∞ Final exam 25% • Attendance*

• Both midterm and final may have written and a practical (computer) parts. Exams are closed-book. A cheat-sheet is allowed (midterm: 1p., final: 2pp). Missed exams can be made up only if the absence is excused (see below). Exam grades may be contested in person or in writing up to one week after receiving the graded exam.

**You are allowed one unexcused absence. After that, every unexcused absence will result in a grade deduction of 3 percentage points, up to a maximum of 9 percentage points. RPI attendance policy requires excuses be validated through the Student Experience Office (4th fl Academy Hall x8022, se@rpi.edu).*

‡Please turn in homework on paper at the beginning of class on the day due unless otherwise specified (note: many homeworks will be turned in electronically). Late homework will be accepted with a 10% penalty for each weekday late for up to 5 weekdays late. Thereafter, late homework is accepted until the last day of classes with a 50% penalty. Homework grades can be contested in person or in writing up to one week after receiving the graded homework, but only if the homework was turned in on time.

∞Term projects are usually done in teams of two. Outside reading is required. Term projects consist of slides and an oral presentation. ***Students enrolled in BIOL 6420*** *will do term projects on their own instead of in teams, and must deliver a written report on their work*

ACADEMIC DISHONESTY: *The Rensselaer Handbook of Student Rights and Responsibilities and The Rensselaer Graduate Student Supplement define various forms of Academic Dishonesty and procedures for responding to them. All forms are violations of the trust between students and teachers. Student-teacher relationships are built on trust. For example, students must trust that teachers have made appropriate decisions about the structure and content of the courses they teach, and teachers must trust that the assignments that students turn in are their own performance. Acts that violate this trust undermine the educational process.*

The Rensselaer Handbook of Student Rights and Responsibilities and The Rensselaer Graduate Student Supplement define various forms of Academic Dishonesty and you should make yourself familiar with these. In this class, all assignments that are turned in for a grade must represent the student's own work. In cases where help was received, or teamwork was allowed, a notation on the assignment should indicate your collaboration. Submission of any assignment that is in violation of this policy will result in a penalty. If found in violation of the academic honesty policy, students may be subject to two types of penalty. The instructor administers an academic [grade] penalty and the student is reported to the Dean of Students or the Dean of Graduate Education as appropriate. The first violation results in 0 grade for that assignment. The second violation results in failure of the course. If you have any questions concerning this policy before submitting an assignment, please ask for clarification.

Learning objectives for BIOL/BCBP 4550

1. Students will be able to critically assess the quality of a protein structure model.
2. Students will demonstrate a thorough understanding of energy calculations for molecular modeling, analysis, and simulation.
3. Students will be able to communicate in the language of bioinformatics on the subject of protein structure and classification.
4. Students will be able to navigate the protein data bank and understand relevant protein data structures.

Additional Learning objective for BIOL/BCBP 6420

5. Students will be able to understand and synthesize information from the molecular modeling literature.

BIOL4550/6420 Molecular Modeling Spring '21

Meets Tue, Fri 8-9:50 AM remote

#	Date	Topic*	
1	Tue, Jan. 26	**Intro to proteins, structure, modeling and MOE: MOE tour tutorial**	cw
2	Fri, Jan. 29	**Where do protein structures come from?**	cb
3	Tue, Feb. 2	**Protein classification**	cb
4	Fri, Feb. 5	**Structural homology**	cb
5	Tue, Feb. 9	**MOE to study barnase/barstar interactions**	cw
6	Fri, Feb 12	**Molecular dynamics**	cw
7	Tue, Feb 16	**Normal mode analysis**	cw
8	Fri, Feb. 19	**Electrostatic surfaces**	cw
9	Tue, Feb. 23	**Force field**	cw
10	Fri, Feb. 26	**Energy Minimization**	cw
11	Tue, Mar. 2	**Docking and drug discovery**	cw
12	Fri, Mar. 5	**Virtual screening, Random sampling and Replica exchange MD**	cw
13	Tues, Mar. 9	**Review**	cw
14	Fri, Mar. 12	**Mid-term exam**	
15	Tue, Mar. 16	**Dr. Nilesh Banavali: structure-function problems**	cw
16	Fri, Mar. 19	**Dr. Hongmin Li: structure-based drug design**	cw
17	Tue, Mar. 23	**Covalent drugs and fragment-based drug discovery**	cw
18	Fri, Mar. 26	**Protein local structure**	cb
19	Tue, Mar. 30	**Side chain rotamers**	cb
20	Fri, Apr. 2	**Homology modeling**	cb
21	Tue, Apr. 6	**Voids and waters**	cb
22	Fri, Apr. 9	**Validation of models**	cb
23	Tue, Apr. 13	**Phylogenetic analysis**	cb
24	Fri, Apr. 16	**Quaternary structure**	cb
25	Tue, Apr. 20	**Modeling nucleic acids**	cb
26	Fri, Apr. 23	**Protein design workshop**	cb
27	Tue, Apr. 27	**Student presentations**	
28	Fri, Apr. 30	**Review**	cb
	TBD	**Final exam**	

* course website on lms.

Grading criteria for BIOL/BCBP 4550 95-100: A, 90-94:A-, 85-89:B+, 80-84:B, 75-79:B-,70-74:C+,65-69:C,60-64:C-, 55-59:D+,50-54:D,0-49:F.
Grading criteria for BIOL/BCBP 6420 95-100: A, 90-94:A-, 85-89:B+, 80-84:B, 75-79:B-,70-74:C+,65-69:C,60-64:C-, 0-59:F.

COVID-19 related policy:

RPI is committed to the health and safety of all students. RPI will continue to monitor any new developments with COVID-19 and determine a course of action that will uphold the well-being of students while maintaining a quality educational experience.