BIOL 4550/6420, Molecular Modeling. SPRING 2017

This course covers the theory and practice of molecular modeling, including force fields, energy minimization, molecular dynamics, homology modeling, modeling of protein structure based on experimental data, docking and drug discovery.

**Place:** SAGE 4510 **Time:** 8-9:50 T,F **Office hours:** W 2:30-3:30.

<table>
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<tr>
<th>Instructor</th>
<th>Chunyu Wang</th>
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<td>Website</td>
<td>RPI LMS</td>
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**Recommended but not required TEXT:** [Z&B]
Marketa Zvelebil & Jeremy Baum. "Understanding Bioinformatics"
Required readings will be posted on the website.

**REQUIRED SOFTWARE:** MOE (Molecular Operating Environment, www.chemcomp.com)
Installed in the classroom and VCC south. VCC south computers are accessible 24/7. VMD and NAMD -- freeware. Install on your own from http://www.ks.uiuc.edu/Development/

**GRADING:** Homework 30%‡  Midterm exam 20%*  
Student presentation 20%*  Final exam 20% 
In-class exercises, participation, attendance: 10%*  

* 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.

*Student presentation will be based on primary protein modeling literature. Outside reading is required. Term projects consist of an oral presentation using powerpoint.

**BFMB majors taking this course for Culminating Experience credit requires receiving a B or better in the course.**

**ACADEMIC DISHONESTY:** See Academic Dishonesty in The Rensselaer Handbook of Student Rights and Responsibilities. Any student committing an act of plagiarism will automatically receive an F for the course and the violation will be reported to the Dean of Students Office.
Learning objectives

1. Students will be able to critically assess the quality of a protein structure model as demonstrated by completing homework assignments and answering questions on an exam.
2. Students will demonstrate a thorough understanding of energy calculations for molecular modeling, analysis, and simulation by completing homework assignments and answering questions on an exam.
3. Students will be able to communicate in the language of molecular modeling on the subject of protein structure and dynamics as demonstrated by a written and oral presentation and answering questions on an exam.
4. Students will be able to navigate the protein data bank and understand relevant protein data structures by completing in-class exercises and completing homework assignments.
# Date | Topic*
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1 Tue, Jan. 17 | Intro to proteins, structure and modeling and MOE: MOE tour tutorial
2 Fri, Jan. 20 | Electrostatic surfaces
3 Tue, Jan. 24 | MOE workshop: Barnase barstar interaction
4 Fri, Jan. 27 | Force field
5 Tue, Jan. 31 | Energy Minimization
6 Fri, Feb. 3 | Molecular Dynamics
Tue, Feb. 7 | Homology model 1: sequence alignment, taught by Prof. Chris Bystroff (CB)
7 Fri, Feb. 10 | Homology model 2 (CB): manual model building
8 Tue, Feb. 14 | Homology model 3 (CB): automated homology Modeling
9 Fri, Feb. 17 | Homology model 4 (CB): remodeling
10 Tue, Feb. 21 | No class: Monday schedule
11 Fri, Feb. 24 | Homology model 5 (CB): Model validation
12 Tue, Feb. 28 | Mid-term
13 Fri, Mar. 3 | Modeling with experimental methods
14 Tue, Mar. 7 | Survey of protein structures
15 Fri, Mar. 10 | Normal mode analysis
March 14, 17 | No class: spring break
16 Tue, Mar. 21 | Monte Carlo
17 Fri, Mar. 24 | Docking and drug discovery
18 Tue, Mar. 28 | Protein and loop design by CB
19 Fri, Mar. 31 | Replica exchange MD: method
20 Tue, Apr 4 | Replica exchange MD: application to Abeta
21 Fri, Apr 7 | Transmembrane proteins
22 Tue, Apr 11 | Student presentation
23 Fri, Apr. 14 | Student presentation
24 Tue, Apr. 18 | Guest lecture by Dr. Nilesh Banavali, Wadsworth Center
25 Fri, Apr. 21 | Student presentation
26 Tue, Apr. 25 | Student presentation
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<tr>
<td>Fri, Apr. 28</td>
<td><strong>Guest lecture on industrial drug discovery by Dr. Mihir Mandal from Merck</strong></td>
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<td>Tue, May 2</td>
<td>Review</td>
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<td>Mon, May 8</td>
<td>Final exam</td>
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*This is a tentative schedule, which may be subject to change without notice.*