BIOL 4550, Bioinformatics II, Molecular Modeling. SPRING 2012

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

Place: Jonsson-Rowland Science Center Rm 2C13 **Time**: 10-11:50 T,F **Office hours**: W 10-12.

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Web sites: http://www.bioinfo.rpi.edu/bystrc/courses/biol4540.html

REQUIRED TEXT: [Z&B]

Marketa Zvelebil & Jeremy Baum. "Understanding Bioinformatics"
Garland Science Textbooks, 2007. ISBN: 0-8153-4024-9
Other required readings will be posted on the website.

REQUIRED SOFTWARE: MOE (Molecular Operating Environment, www.chemcomp.com)

Install from disk on first day of class. A license key will be provided. JMOL -- freeware. Install on your own from http://jmol.sourceforge.net/download/

GRADING: Homework 30%‡ Midterm exam 20%•,
Term project 20%∞ Final exam 20% •
In-class exercises, participation, attendance: 10%*

• Both midterm and final have a written and a practical (computer) part. 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 and programming are required. Term projects consist of a written report and an oral presentation. Persons taking this course for **Culminating Experience** credit must state this at the start of the term and must do their term projects individually instead of in a team. 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 bioinformatics on the subject of protein structure and classification 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.

BIOL4550 Bioinformatics II Spring '12

Meets Tues, Fri 10:00-11:50AM J-ROWL 2C13

Lecture	Date	Topic	Reading (Z&B)	Homework* & exercises.
1	Tue, Jan. 24	**Intro to proteins and amino acid structure**	25-43	Ex 1.1
2	Fri, Jan. 27	**Where do protein structures come from?**		Ex 2.1
3	Tue, Jan. 31	**Protein classification. TOPS drawings.**	567-582	Ex 3.1-3
4	Fri, Feb. 3	**Rotation matrices. Least Squares. Superposition.**		Ex 4.1
5	Tue, Feb. 7	**MOE workshop 1: Building small molecules**		HW 1 due
6	Fri, Feb. 10	**MOE workshop 2: Secondary structure**		Ex 5.1
7	Tue, Feb 14	**Comparative modeling 1: Alignment, Deletions**		HW 2 due
8	Fri, Feb. 17	**Comparative modeling 2. Insertions**	537-565	
9	Tue, Feb. 21	**Comparative modeling 3. Outgaps.**		HW 3 due
10	Fri, Feb. 24	**Comparative modeling 4. Voids and waters.**		HW 4 due
11	Tue, Feb. 28	**Comparative modeling 5. Evaluation.**		HW 5 due
12	Fri, Mar. 2	**Comparative modeling 6. Interpetation and significance.**		HW 6 due
13	Tue, Mar. 6	**Review.**		HW 7 due
14	Fri, Mar. 9	**Midterm Exam**		
		Spring Break		
15	Tue, Mar. 20	**Molecular Surfaces. Poisson-Boltzman equation**	580-587	
16	Fri, Mar. 23	**Ab initio methods and threading**	521-537	HW4
17	Tue, Mar. 27	**Force fields , Energy Minimization**	700-719	
18	Fri, Mar 30	**Molecular Dynamics 1**		
19	Tue, Apr 3	**Molecular Dynamics 2**		HW4 due
20	Fri, Apr 6	guest lecture Nilesh Banavali		
21	Tue, Apr 10	**Normal mode analysis**		HW5
22	Fri, Apr. 13	**Docking 1**	585-593	
	Tue, Apr. 17	no class		
23	Fri, Apr. 20	**Docking 2**		HW5 due
24	Tue, Apr. 24	**Protein Design 1**		HW6
25	Fri, Apr. 27	**Protein Design 2**		
26	Tue, May. 1	**Review**		HW6 due
27	Fri, May. 4	**Student presentations**		
28	Tue, May. 8	**Final Exam**		

* Upload MOE homework to http://www.bioinfo.rpi.edu/bystrc/courses/biol4550/homework.html