

## **BIOL 4550, Bioinformatics II, Molecular Modeling. SPRING 2004**

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

**Place:** Jonsson-Rowland Science Center Rm 2C13

**Time:** Wednesday 5:30-8:30pm

**Instructors:** Chris Bystroff

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**Office Hours:** Wed. 11-12am 2C13

**Web site:** <http://www.bioinfo.rpi.edu/~bystrc/courses/bioinf2/>

[http://bioinf45.bio.rpi.edu/Bioinfo2\\_2004/](http://bioinf45.bio.rpi.edu/Bioinfo2_2004/)

REQUIRED TEXT:

**“Bioinformatics: Genes, Proteins and Computers”**

**by Christine A. Orengo et al, 2003.**

Other required readings will be placed on reserve or online.

GRADING:

Homework (incl spelunking assign.) 25%

Midterm Exam 25%

Term project 20%

Final exam: 25%

Class Participation 5%

Please turn in homework on paper at the beginning of class unless otherwise specified. Both exams have written and practical parts.

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#	Date	Topic	Reading (Orengo)	Instructor/ homework
1	1/14	Introduction to molecular structures. X-ray and NMR. PDB website. Protein Folding.	handouts	Chris
2	1/21	Protein Structure; Molscript; Insight2; MAGE; Molecular Spelunking; Secondary structure prediction.	Sect. 9.3 Reserve reading (required)	Susan
3	1/28	Mathematics of rotation; Least squares superposition. Structure-based alignment. Structural classification.	Ch 6, 7	HW 1 Due Chris
4	2/4	Molecular mechanics and introduction to model building (ab initio& threading)	Ch. 9, Ch. 8	Susan
5	2/11	Homology modeling using Insight2. Defining a basis set.	Ch. 8	Spelunking Assignment Due. Susan
6	2/18	Homology modeling using Insight2. Modeling splice points and loops.		HW 2 Due Chris
7	2/25	<b>Midterm</b>		Midterm
8	3/3	Energy Minimization, Molecular dynamics, Monte Carlo and simulated annealing	handouts	Chris choose term projects
9	3/10	<b>**NO CLASS SPRING BREAK**</b>		
10	3/17	Ligand issues in modeling; Small molecule model building.	Ch 13	Susan
11	3/24	Molecular surfaces, Electrostatic maps, the hydrophobic effect.	handouts	HW 3 due Chris
12	4/7	Sidechain modeling and protein design.	handouts	Chris
13	3/31	<b>**NO CLASS GM WEEK**</b>		
14	4/14	Flexible Docking, drug design.	Ch 13	HW4 due Susan
15	4/21	Statistical and experimental validation of molecular models.		Susan
16	4/28	Student Presentations		Term project due
	5/5 ?	<b>Final Exam</b>		