BIOL 8804B / BIOL 4804A / CHEM 4804A
Spring, 2007

Course Syllabus

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Course objectives:

- Give students practical experience in building and evaluating molecular models
- Give students a thorough understanding of the basic principles behind molecular mechanics force fields and algorithms
- Give students practical experience in molecular graphics, homology modeling, energy minimization and molecular dynamics)
- Deepen students' understanding of principles of macromolecular structure, and of macromolecular structure – function relationships

To achieve these objectives, the course will contain a mixture of lectures, "cookbook" laboratory exercises, reading assignments from the text and from the literature, discussion sections, and written examinations.

MS and PhD students will also carry out an independent term project and will turn in a 10-20 page report on this project by the end of the semester; undergraduates are encouraged, but not required, to carry out an independent term project.

Texts: *Molecular Modelling: Principles and Applications, Second Edition*
Andrew R. Leach
Prentice–Hall (2001)

Molecular Modeling and Simulation: An Interdisciplinary Guide
Tamar Schlick
Springer (2002)

(I suggest you buy only one, but team up with someone who has bought the other.)

Grading (Undergrads):

Written exams		70%
Exam 1	15%	
Exam 2	20%	
Pop quizzes	5%	
Final exam	30%	
Homework, classroom participation and laboratory exercises		30%
TOTAL		100%

Grading (Graduate students):

Written exams		50%
Exam 1	10%	
Exam 2	15%	
Pop quizzes	5%	
Final exam	20%	
Homework, classroom participation and laboratory exercises		25%
Term project		25%
TOTAL		100%

General policies:

Attendance is mandatory at all Tuesday and Thursday classes.
Students are allowed one unexcused absence during the semester.

Each additional unexcused absence will result in loss of one full letter grade from the "Classroom Participation" grade

Late homework and labwork:

1 day: loss of one full letter grade for that particular assignment
2 days: loss of two full letter grades for that particular assignment
3 days: labwork not accepted; loss of all credit for that particular assignment

Makeup exams: there will be no makeup exams.

Exceptions:

In exceptional cases, I may be persuaded to allow someone to take a makeup exam, but only if it is arranged at least 48 hours before the exam.

Any of the above requirements can be waived in case of: (1) serious illness or injury; (2) the death of an immediate family member; or (3) the serious illness or injury of a spouse or a dependent child.

Honor Code:

I take intellectual honesty very seriously, and any violation of the conditions below will result in immediate expulsion from the course with a grade of "F".

– Stephen C. Harvey

I. In order to truly understand the material you are studying, and in order to avoid any student taking unfair advantage of any other, it is absolutely essential that none of you copy or use the results of any one else's work. Throughout most of the semester, you will be encouraged to collaborate with one another, and the free exchange of information and ideas is encouraged, but you are required to complete all assignments yourself, without copying or using the results of anyone else's work. All quizzes and exams must, of course, be completed without consulting anyone else or using any unauthorized materials ("cheat sheets"). Your final report should include appropriate citations to other people's contributions.

II. All students in this course are bound by the conditions of the Georgia Tech Honor Code. A copy of the Honor Code can be found at http://www.deanofstudents.gatech.edu/Honor. The Graduate Appendix to the Honor Code is of sufficient importance that a copy of it is appended here:

Graduate Appendix to the Honor Code

1. Preamble: The Honor Code recognizes that graduate students are involved in research and scholarly activities which occur outside the classroom. Integrity and academic honesty are as fundamental to research and scholarly activity as they are to classroom activity. Therefore, this Appendix to the Honor Code is adopted to pertain to the academic activities of graduate students which occur outside of the classroom.

2. Scholarly Misconduct: Scholarly misconduct refers to misconduct which occurs in research and scholarly activities outside of the classroom. It can include plagiarism, among other things. The consequences of scholarly misconduct are governed by Institute policy. The following definitions are taken from the Institute's Policy on Scholarly Misconduct.

"Misconduct" or "scholarly misconduct" is the fabrication or falsification of data, plagiarism, or other practice that seriously deviates from those that are commonly accepted within the academic or research community for proposing, conducting or reporting research or scholarly activity. It does not include honest error or honest differences in interpretation or judgments of data.

"Plagiarism" is the act of appropriating the literary composition of another, or parts or passages of his or her writings, or language or ideas of the same, and passing them off as the product of one's own mind. It involves the deliberate use of any outside source without proper acknowledgement. Plagiarism is scholarly misconduct whether it occurs in any work, published or unpublished, or in applications for funding.

Allegations involving scholarly misconduct fall under the Institutes Policy on Scholarly Misconduct. This document details the procedures involved with reporting allegations and with the handling of cases. All graduate students are encouraged to become familiar with this policy, which is available from the Office of the Provost.

BIOL 8804B / CHEM 4804B Schedule Spring 2006

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	Date	Lecture / Lab
1	Tue Jan 9	Course introduction; Review of macromolecular structure
2	Thu Jan 11	**QUIZ ON MACROMOLECULAR STRUCTURE**
3	Tue Jan 16	Thermodynamics I: The first law; thermochemistry
4	Thu Jan 18	Thermodynamics II: The second law; entropy; free energy
5	Tue Jan 23	Thermodynamics III: Equilibrium; Nonequilibrium systems & coupled reactions; Boltzmann relation
6	Thu Jan 24	Review for exam; Introduction to molecular modeling: Goals and history
7	Tue Jan 30	**EXAM 1**
8	Thu Feb 1	Representing and viewing molecules on a computer
9	Tue Feb 6	Characterizing molecules and models
10	Thu Feb 8	Force fields I: Calculating the conformational energy
11	Tue Feb 13	Force fields II: Parameterization
12	Thu Feb 15	Algorithms I: Grid search and energy minimization
13	Tue Feb 20	Algorithms II: Molecular dynamics: The basics
14	Thu Feb 22	Force fields III: Electrostatics: The basics
15	Tue Feb 27	Algorithms III: Molecular dynamics: The details
16	Thu Mar 1	Homology modeling I
17	Tue Mar 6 *	Lab and review day
18	Thu Mar 8	Force fields IV: Electrostatics: The complications
19	Tue Mar 13	Review for exam
20	Thu Mar 15	**EXAM 2**
	Tue Mar 20	SPRING BREAK
	Thu Mar 22	SPRING BREAK
21	Tue Mar 27	Homology modeling II
22	Thu Mar 29	Simplifications I: Implicit solvation models
23	Tue Apr 3	Simplifications II: Coarse-grain models
24	Thu Apr 5	Simplifications III: Lattice models
25	Tue Apr 10	Algorithms IV: Monte Carlo; Langevin dynamics; Brownian dynamics; Normal mode analysis
26	Thu Apr 12	Algorithms V: Biased searches; Free energy methods; Conformational transitions
27	Tue Apr 17	Algorithms VI: Structure refinement: X-ray crystallography, NMR, and Cryo-electron microscopy
28	Thu Apr 19	Structure prediction and the folding problem
29	Tue Apr 24	Future directions
30	Thu Apr 26	Review for final exam
	Tue May 1	**FINAL EXAM**

***** SCH out of town