BIOL 8104 Course Syllabus

Class	Date	Lecture / Lab
1	Tue Jan 10	Introduction: Molecular modeling as a laboratory technique; order of magnitude estimates
2	Thu Jan 12	**QUIZ ON MACROMOLECULAR STRUCTURE**
3	Tue Jan 17	Thermodynamics I: The first law; thermochemistry
4	Thu Jan 19	Thermodynamics II: The second law; entropy; free energy
5	Tue Jan 24	Thermodynamics III: Equilibrium; free energy changes in nonequilibrium systems; coupled reactions
6	Thu Jan 26	Review of macromolecular structure
7	Tue Jan 31	**EXAM 1**
8	Thu Feb 2	Overview of molecular modeling: Goals and history
9	Tue Feb 7	Viewing molecules on a computer: Introduction to VMD
10	Thu Feb 9	Cartesian and internal coordinates; Potential energy surface of butane; The Boltzmann factor
11	Tue Feb 14	Force fields I: Bonds, angles, torsions, van der Waals forces
12	Thu Feb 16	Algorithms I: Conformational searches: grid search, minimization and molecular dynamics (MD)
13	Tue Feb 21	Modeling small molecules: MOE I (with Pete Ludovice)
14	Thu Feb 23	Modeling small molecules: MOE II (with Pete Ludovice)
15	Tue Feb 28	Force fields II: Problem set on bonds, angles, torsions, van der Waals and the partition function
16	Thu Mar 2	NAMD tutorial 1: Basics (§1.1–1.7)
17	Tue Mar 7	The first protein MD simulation: McCammon *et al. Nature 267:*585-590 (1977).
18	Thu Mar 9	NAMD tutorial 2: Analysis of equilibrium properties (§2.1–2.4)
	Tue Mar 14	Review for exam
19	Thu Mar 16	**EXAM 2**
	Tue Mar 21	SPRING BREAK
	Thu Mar 23	SPRING BREAK
20	Tue Mar 28	Force fields III: Electrostatics and the treatment of solvent – Basics
21	Thu Mar 30	Force fields III: Electrostatics and the treatment of solvent – The complications
	Mon Apr 3	Molecular Simulations Symposium Honoring Martin Karplus – Emerson Center at Emory
22	Tue Apr 4	Reduced representations I: Introduction; Lattice models; A simple model for protein folding
23	Thu Apr 6	Reduced representations II: Models for DNA and RNA
	Fri Apr 7	Frontiers in Macromolecular Simulations – University of Alabama at Birmingham
	Sat Apr 8	Frontiers in Macromolecular Simulations – University of Alabama at Birmingham
24	Tue Apr 11	Algorithms III: Modeling conformational transitions with biased MD methods
25	Thu Apr 13	MD Simulations on the Assembly of RNA-Protein Complexes: U1A–ST2 RNA (with David Beveridge)
26	Tue Apr 18	Algorithms IV: Monte Carlo and replica exchange
27	Thu Apr 20	The protein folding problem
28	Tue Apr 25	Algorithms V: Modeling methods in structure refinement: crystallography, NMR, cryo-electron microscopy
29	Thu Apr 27	Future challenges in molecular modeling; Review for exam
	Tue May 2	**FINAL EXAM**