Preparation for the exam 2

Chem112L, Spring 2009 **Exam dates: Monday, June, 8 and Wednesday, June 10**

This exam focuses on structure determination by modeling and NMR, protein-ligand interactions as studied by spectrophotometry, and crystallization / diffraction analysis of macromolecules. I expect that you know the basic material from the three previous experiments as well. I intend to have a mix of knowledge-showing essay-type, problem-solving, and multiple-choice questions. Knowledge of the following helps you in preparing for the exam:

1. Physical principles behind each of the molecular process
    a. Forces determining conformations of small molecules
    b. Ligand binding to macromolecules
    c. Protein crystallization

2. Physical principles behind each of the observation/detection methods
    a. X-ray diffractiometry
    b. UV absorption spectroscopy, design of UV-vis spectrophotometer
    d. Nuclear magnetic resonance detection of nuclei: chemical shift
    e. NMR as a tool to study molecular structures: coupling, TOCSY, NOE
    f. Molecular modeling with computers: MC, MD, and conformational analysis

3. Theoretical description of conformational equilibria, and ligand binding
    a. Estimation of thermodynamic parameters from experimental data
    b. Dissociation constant in relation to equilibrium concentrations
    c. The harmonic oscillator as a simple model for the chemical bond
    d. Description of molecular structures in terms of potential energy surfaces
    e. Minimization, conformational search, and Monte Carlo sampling
    f. Calculation of observable macroscopic properties from properties of components
    g. Partition function and it's relationship to average energy
    h. Relationships between free energy, enthalpy, entropy and heat capacity

4. Structural and functions concepts pertaining to ligand binding and protein function
    a. Biological function and catalytic mechanism of lysozyme
    b. Structure of peptides and proteins
    c. Solvatochromic shifts in UV-Vis spectra

5. Instrumentation
    a. Basic design and operation of a X-ray diffractiometers and synchrotrons
    b. Basic design and operation of a dual-beam UV spectrophotometer
    c. Basic design and operation of a FT-NMR spectrometer

6. Broader applications of methods covered; other approaches to study these phenomena
    a. Using circular dichroism and mass spectrometry to study ligand binding
    b. Other methods to ligand binding
    c. Other methods to study conformation of small molecules

7. Practical aspects of each of the experiments and computations
    a. Why such wavelengths and cuvettes

c. Why such concentrations, pH, salts, buffers, etc
d. Why such simulation parameters and computational protocols

8. Data analysis.
a. Understand why we used such model equations for fitting
b. Understand the meaning of each of the fitting parameters
c. Understand the measures of quality of data and fitting
d. Understand the workflow of scientific data analysis programs such as *Mathematica*
e. Understand how to analyze 2D NMR spectra
f. Understand how to interpret 2D X-ray diffraction data
g. Understand how to interpret 3D electron density maps

9. Miscellaneous
a. How to derive equations for association/dissociation equilibrium
b. How to interpret and use molecular force fields
c. How to estimate fitting parameters: you may need a calculator
d. How to make solutions: you may need a calculator

Answers to many of the questions require substantial thinking. Memorizing all the material may not be the best way to study for this exam.