

Preparation for the exam 1

Chem112L, Spring 2008

Exam dates: Monday, May 12, and Tuesday, May 13

This exam focuses on structure determination by modeling and NMR, protein-ligand interactions as studied by spectrophotometry, and study of protein folding by circular dichroism. 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. Forces determining folding of macromolecules
 - b. Role of entropy in protein folding
 - c. Ligand binding to macromolecules
 - d. Protein ionization and its relevance to mass spectrometry
2. Physical principles behind each of the observation/detection methods
 - a. Circular dichroism, design of a spectropolarimeter
 - b. UV absorption spectroscopy, design of UV-vis spectrophotometer
 - c. Nuclear magnetic resonance detection of nuclei: chemical shift
 - d. NMR as a tool to study molecular structures: coupling, TOCSY, NOE
 - e. 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
4. Structural and functions concepts pertaining to ligand binding and protein folding
 - a. Biological function and catalytic mechanism of lysozyme
 - b. Structure of peptides and proteins
 - c. Chiral and achiral molecules
 - d. Protein folding diseases: prions
5. Instrumentation
 - a. Basic design and operation of a spectropolarimeter
 - 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 to study ligand binding
 - b. Other methods to study protein folding and ligand binding
 - c. Other methods to study conformation of small molecules
7. Practical aspects of each of the experiments
 - a. Why such wavelengths and cuvettes
 - b. Why such concentrations, pH, salts, buffers, etc

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*

9. Miscellaneous

- a. How to estimate fitting parameters: you may need a calculator
- b. 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.