Chem112L, Spring 2006

Preparation for the exam 1:

This exam focuses on the following three experiments: structure determination by modeling and NMR, ligand binding equilibrium, and multisubstrate enzyme kinetics. 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. Binding of small molecules to macromolecules
   c. Enzyme catalysis

2. Physical principles behind each of the observation/detection methods
   a. UV-Vis absorption spectroscopy and solvatochromic shifts
   b. Nuclear magnetic resonance detection of nuclei: chemical shift, coupling, NOE
   c. Measurement of equilibrium and kinetics by these methods
   d. Molecular modeling with computers: MC, MD, and conformational analysis

3. Thermodynamic description of conformational equilibria, and ligand binding
   a. Dissociation constant in relation to equilibrium concentrations
   b. Dissociation constant in relation to rate constants in a reversible reaction
   c. Estimation of thermodynamic parameters from experimental data

4. Quantum mechanical description of structure and reactivity
   a. Simple models: the hydrogen atom and harmonic oscillator
   b. Description of molecular structures in terms of potential energy surfaces
   c. Description of chemical reactivity in terms of potential energy surfaces
   d. Zero point energies and the kinetic isotope effect
   e. Tunneling

5. Practical aspects of each of the experiments
   a. Why such wavelengths
   b. Why such concentrations, pH, salts, buffers, etc
   c. Why such cuvettes

6. Data analysis
   a. Understand the meaning of all the data observed
   b. Understand why we used such model equations for fitting
   c. Understand the meaning of each of the fitting parameters
   d. Derivation of equations that relate observables to concentrations: equilibrium process
   e. Derivation of equations that relate observables to concentrations: enzyme kinetics

7. Miscellaneous
   a. Application of these methods to other problems in chemistry
   b. Application of other methods to study these phenomena
   c. How to estimate fitting parameters: you may need a calculator
   d. How to make solutions: you may need a calculator