Preparation for the exam 1

Chem112L, Spring 2009 **Exam dates: Monday, May 11, and Tuesday, May 12**

This exam focuses on mass spectrometry, enzyme kinetics, and study of protein folding by circular dichroism. 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. Protein ionization and its relevance to mass spectrometry
    b. Protein folding, especially role of entropy in it
    b. Enzyme catalysis and inhibition

2. Physical principles behind each of the observation/detection methods
    a. Polarimetry and circular dichroism
    c. Separation of molecules based on m/z values; protein identification
    d. Measurement of reaction rates by UV-Vis spectrophotometry

3. Theoretical description of conformational equilibria, and chemical reactions
    a. Estimation of thermodynamic parameters from experimental data
    b. Dissociation constant in relation to equilibrium concentrations
    c. Rate constants in relation to equilibrium constant
    d. Steady state approximation for consecutive reactions
    e. Transition state stabilization concept in enzyme catalysis
    f. Description of reactions via intersecting potential energy surfaces
    g. The energy levels and wave functions of quantum harmonic oscillator
    h. Kinetic isotope effect and tunneling in chemical reactions
    i. Enthalpy and heat capacity change in chemical reactions

4. Structural and functions concepts pertaining to kinetics, mass spectrometry 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
    e. Structure and function of heme-containing proteins
    f. Chemistry of NAD-dependent dehydrogenases

5. Instrumentation
    a. Basic design and operation of a spectropolarimeter
    b. Basic design and operation of a dual-beam UV spectrophotometer
    c. Ionization/vaporization methods for small molecule MS
    d. Ionization/vaporization methods for macromolecule MS
    e. Basic design and operation of a ESI mass spectrometer
    f. Comparison of different mass analyzers

6. Broader applications of methods covered; other approaches to study these phenomena
    a. Using circular dichroism to monitor structural changes in protein
    b. Other methods to study protein folding
    c. Other methods to study enzyme catalysis

    d. Applications of mass spectrometry in proteomics

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
    c. How to derive one and two-substrate enzyme kinetic equations
    d. How to derive kinetic equations with one substrate and inhibitor
    e. How to derive equations for protein unfolding equilibrium
    f. How to derive equations that describe temperature-dependence of equilibrium constants

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