

Structural Bioinformatics
Fall 2007
Course Syllabus

Graduate School of Biomedical Sciences
University of Medicine and Dentistry of New Jersey

Meeting Times and Dates (by campus)

Newark: Monday 1:00 PM to 4:00 PM in ACS/Bioinformatics Facility (MSB C-632)

Piscataway: Tuesday 1:00 PM to 4:00 PM in V12 Teaching Lab

NOTE: The week of August 27th will be the first week that class meets!

Attendance is mandatory, unless you have a University sanctioned excuse (e.g. medical or legal).

Instructors:

John E. Kerrigan, Ph.D., Course Coordinator

Phone: (732) 235-4473; Email: kerrigje@umdnj.edu

Webpage: <http://www2.umdnj.edu/~kerrigje/index.htm>

Course Webpage: http://www2.umdnj.edu/~kerrigje/structbio_II.htm

Sandhya Kortagere, Ph.D.

Phone: (732) 235-0181; Email: kortagsa@umdnj.edu

Vladyslav Kholodovych, Ph.D.

Phone: (732) 235-3229; Email: kholodvl@umdnj.edu

Narayanan Ramasubbu, Ph.D.

Phone: (973) 972-0704; Email: ramasun1@umdnj.edu

Textbook: Andrew R. Leach, (2001) "Molecular Modelling, Principles and Applications" 2nd Ed. Prentice Hall (Pearson Education), New York, NY

ISBN 0-582-38210-6

<http://www.pearsoneduc.com>

Course Topics/Outline:

Introduction: Review of Unix Commands (Kerrigan) (8/27 – Newark; 9/4 – Piscataway)

September 3rd - Labor Day Week, No Class in Newark

September 4th – Class in Piscataway.

I. Experimental Three Dimensional Structure Determination (Ramasubbu) (9/10)

1. X-Ray Crystallography
2. NMR
3. The Protein Data Base and the PDB File Format

II. Review of Macromolecular Structure (Kerrigan) (9/17 & 9/24)

- A. Proteins
 1. Primary Structure
 2. Secondary Structure
 3. Tertiary Structure
 4. Quaternary Structure
- B. Nucleic Acids
 1. DNA – A, B, Z forms
 2. RNA
- C. Viewing Tools
 1. Rasmol
 2. DeepView
 3. VMD
- D. Graphics Tools
 1. Molscript
 2. Raster3D

III. Homology Modeling (Kerrigan) (10/1 & 10/8)

- A. Sequence Alignment
 1. Multiple Sequence Alignments
 2. BLAST, FASTA, PAM
 3. EMBOSS
 4. Databases (NCBI)
- B. Homology Model Programs
 1. SwissProt (submission to a web resource)
 2. Modeller (Sali's popular model builder)

IV. Introduction to Force Fields and Modeling (Kortagere) (10/15)

- A. Intro to Force Fields
- B. Building small molecules
- C. Building small peptides/nucleic acids

V. Molecular Dynamics (Kortagere) (10/22 & 10/29 & 11/5)

- A. Energy minimization (theory and applications)
- B. Molecular Dynamics
 1. Theory
 2. Applications using AMBER and CHARMM force fields
- C. Monte Carlo techniques (theory and applications).

VI. Docking (Kholodovych) (11/12 & 11/19)

- A. Simulated Annealing

- 1. Autodock
- B. Genetic Algorithms
 - 1. Autodock
 - 2. FlexX
 - 3. Gold
- C. Other Methods
 - 1. Tabu
 - 2. DOCK (spheres vs grids)
 - 3. FTDOCK (Docking small/medium sized polypeptides to proteins)
- D. Scoring Methods
 - 1. Simple Interaction Energies
 - 2. GB/SA scoring (implicit solvation)
 - 3. CScore (consensus scoring algorithms)

VI. Structure-Based Drug Design Strategies (Kholodovych) (11/26 & 12/3)

- A. Simple Structure Activity Relationships
- B. “Inside out” and “Outside in”

Note: This is a broad, general outline. New topics may be added and older topics removed by the individual instructors in the course. Each instructor will provide an outline for his or her course section.

Course Assignments/Grading:

Each instructor will have his or her own style of grading/evaluation in the course. This evaluation may be a composite of exams/quizzes, homework, oral presentation, and/or research paper(s). Therefore, each instructor is responsible for establishing a grading format for his or her section of the course.

E-Mail Submission Policy: Reports are to be submitted in either MS Word or PDF (Acrobat) formats to the appropriate instructor listed on the project description. Use your last name and first initial in the filename.

Projects are to be prepared in the format specified by the instructor. Typically, this format will be in some journal manuscript style (i.e. as if you were preparing an actual manuscript for publication). See page 21 of the GSBS Student Handbook for guidelines on preparation of research papers. http://www.umdnj.edu/gsbweb/documents/2004-2005_GSBS_Handbook.pdf

A quick evaluation guide for project reports–

Organization – Did the student follow the journal format/typing instructions?

Presentation – Did the student label charts/graphics clearly? Were tables properly formatted? Were the figures easy to follow? Did the student give an adequate introductory discussion with appropriate literature citations?

Citations – Did the student adequately cite the literature? Were the methods used cited properly?

Content – Did the student explain the data/results in a thorough and convincing manner? Were the conclusions given supported by the data?

Course Policy: Students are expected to abide by the Code of Professional Conduct outlined in the GSBS Student Handbook on page 20 (http://www.umdj.edu/gbsnweb/documents/2004-2005_GSBS_Handbook.pdf). All work is to be independent and original on the part of the student. Assignment deadlines are to be met by the student, no exceptions.

Late Policy: In general, all assignments are to be submitted by the deadlines given by the instructor. *Only the instructor can alter his/her assignment due dates.* The course coordinator will not alter assignment due dates assigned by the instructor. A University sanctioned excuse (i.e. a letter from the Dean is required) is required for all make-up work. Each instructor establishes his or her own late penalties.

Resolution of Disputes: Students are to resolve their differences with the instructor first. If the complaint cannot be resolved at the instructor level, the student should consult the course coordinator before going to the Associate Director of the Informatics Institute (Bruce Byrne, Ph.D., byrne@umdj.edu; phone 7-7788) or the Dean of the Graduate School.