

Structural Bioinformatics I

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

Meeting Times and Dates (by campus) **January 24th is first meeting date!**

Newark: Monday 1:00 PM to 4:00 PM in ACS/Bioinformatics Facility

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

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

Holiday: There will be no class the week of January 17th (MLK Day)

Instructors:

John 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_I.htm

Susan Keenan, Ph.D.

Email: keenanasm@umdnj.edu

Vladyslav Kholodovych, Ph.D.

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

A.R. Srinivasan, Ph.D.

Phone: (732) 445-4619 Email: srini@rutchem.rutgers.edu

William Welsh, Ph.D.

Phone: (732) 235-3234 Email: welshwj@umdnj.edu

Course Outline:

- i. Unix Workshop (Kerrigan, 1/24)
 - I. Introduction to Structure and Bonding (Srinivasan, 1/31)
 - II. Electronic Structure Methods (Srinivasan, 2/7 to 2/18)
 1. ab initio
 2. Semi-empirical
 3. Properties
- Project/Exam Week (Week of February 21st)

- III. Molecular Mechanics (Empirical) (Kholodovych, 2/28)
 - IV. Conformation Searching (Kholodovych 3/7 to 3/14)
Project/Exam Week (weeks of March 21st and March 28th)
 - V. Small Molecule Drug Design Considerations (Keenan, 4/4)
 - 1. Pharmacology Review
 - 2. Intro to SAR
 - VI. Quantitative Structure Activity Relationships (Welsh, 4/11 to 4/29)
Project/Exam weeks (April 25th & May 2nd)
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Evaluation: Your grade will consist of exams/quizzes/problem sets and/or projects at the discretion of the instructor. Each section of the course is counted equally in computing your final grade.

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.umdj.edu/gsbweb/documents/2004-2005_GSBS_Handbook.pdf.

Projects are to be prepared in the format specified in the project description handout. Typically, this format will be in some journal manuscript style (i.e. as if you were preparing an actual manuscript for publication) as assigned by the instructor.

A quick evaluation guide for instructors –

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.umdnj.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 or Dean of the Graduate School.