

Fall Course Announcement: AMS-535

Introduction to Computational Structural Biology and Drug Design

Dr. Robert C. Rizzo

Class schedule and syllabus: <http://www.ams.sunysb.edu/~rizzo> (go to Teaching)

Dear Stony Brook Students and Faculty,

This Fall I be teaching a course entitled "Introduction to Computational Structural Biology and Drug Design" (AMS-535). **No prior knowledge is assumed and all are welcome to attend.**

AMS-535 provides an introduction to the field of computational structure-based drug design. The course aims to foster collaborative learning and will consist of presentations by myself, course participants, and guest lecturers arranged in five major sections as outlined below. Presentations should aim to summarize key papers, theory, and application of computational methods relevant to computational drug design. Grades will be based on the quality of the talks, participation in class discussion, attendance, five quizzes, and a final.

A companion course taught in the Spring (AMS-536, "Molecular Modeling of Biological Molecules") gives hands-on experience in using computational methods discussed in the introductory Fall course. **Students interested in taking the two-semester sequence should plan accordingly** since AMS-535 (Fall) is a prerequisite for AMS-536 (Spring).

This should be a very exciting course.

Sincerely,
Rob Rizzo

Topics to be covered include.

1. Drug Discovery and Biomolecular Structure

Drug Discovery, Chemistry Review, Proteins, Carbohydrates, Nucleic acids
Molecular Interactions and Recognition, Experimental Techniques for Elucidating Structure

2. Molecular Modeling

Classical Force Fields (Molecular Mechanics),
Solvent Models, Condensed-phase Calculations, Parameter Development

3. Sampling Methods

Conformational Space, Molecular Dynamics (MD), Metropolis Monte Carlo (MC)
Sampling Techniques, Predicting Protein Structure, Protein Folding

4. Lead Discovery

Docking as a Lead Generation Tool, Docking Algorithms
Discovery Methods I, Discovery Methods II, Applications

5. Lead Refinement

Binding Energy I. Free Energy Perturbation (FEP)
Binding Energy II. Linear Response (LR), Extended Linear Response (ELR)
Binding Energy III. MM-PBSA, MM-GBSA, Properties of Known Drugs, Property Prediction