Spring Course Announcement: AMS-536

Molecular Modeling of Biological Molecules

Dr. Robert C. Rizzo

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

Dear Stony Brook Students and Faculty,

This Spring I will be teaching a course entitled "Molecular Modeling of Biological Molecules" (AMS-536). I would appreciate you bringing the course to the attention of any students you feel would be interested.

AMS-536 is designed for students who wish to gain hands-on experience modeling biological molecules at the atomic level. In conjunction with the participants' interest, Molecular Mechanics, molecular dynamics, Monte Carlo, Docking (virtual screening), or Quantum Mechanics software packages will be used. Projects will include setup, execution, and analysis. Students will work on individual projects outside of class. Course participants will give presentations relevant to the simulations being performed and a final project report will be required. Familiarity with working in a Unix (Linux) environment is desirable.

Prerequisites are AMS-535 "Introduction to Computational Structural Biology and Drug Design" taught in the Fall semester. Students that have not taken AMS-535 but have a good understanding of Molecular Modeling may request permission to enroll. Grades will be based on attendance, class participation, quality of the presentations, and the final project report.

This should be a very exciting course.

Sincerely,
Rob Rizzo

Examples of student final projects from prior semesters include:

- Molecular Dynamics Simulations of A-DNA to B-DNA Transition with AMBER
- Comparative Homology Modeling of the Catalytic Domains of mTOR and DNA-PK for the Design of Anti-Cancer Agents
- Effects of Run Characteristics on Convergence of Data: How Specific Cycle and Iteration Sequences Effect the Quality of Resultant Data
- Simulating Botulinum Neurotoxin Type A with Constant pH Molecular Dynamics in Generalized Born Implicit Solvent
- Protein Folding of Trpcage Using Generalized Born and Explicit Solvent Molecular Dynamics
- Building a Docking Test Set
- Docking Botulinum Neurotoxin Type E Light Chain with Phosphoramidon: A Structure Based Rational Drug Design Study for Developing Drug Targets for Botulism
- Pharmacophore Searching in HIV protease
- MOE's Docking of Sustiva Analogues as HIV-1 Reverse Transcriptase Inhibitors
- Statistical Study of QSPR of Blood-Brain Partitioning for a Large Set of Drugs