# CS 5984 Algorithms in Structural Bioinformatics
(Spring 2006)

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In the post-genomic era, key problems in molecular biology center on the determination and exploitation of three-dimensional molecular structure and function. This course will discuss the computational techniques for analysing, modeling and predicting the three-dimensional structure of biological molecules. The emphasis will be on algorithmic research for protein structural comparison and molecular docking. Molecular docking can be defined as the computational prediction of the three-dimensional structure of receptor-ligand complexes, where the receptor is a protein and the ligand is either another protein, or a small molecule, or a macromolecule like DNA or RNA. Molecules seldom act alone and the binding of ligand molecules to protein receptors is central to numerous biological processes. Accurate predictive docking methods can provide substantial structural knowledge about complexes, from which functional information could be inferred or experiments could be designed to obtain it. In particular, accurate and efficient protein-small molecule docking algorithm is of fundamental importance to the structure-based drug design, with major potential to develop new therapeutics for AIDS, cancer, infectious and other diseases.
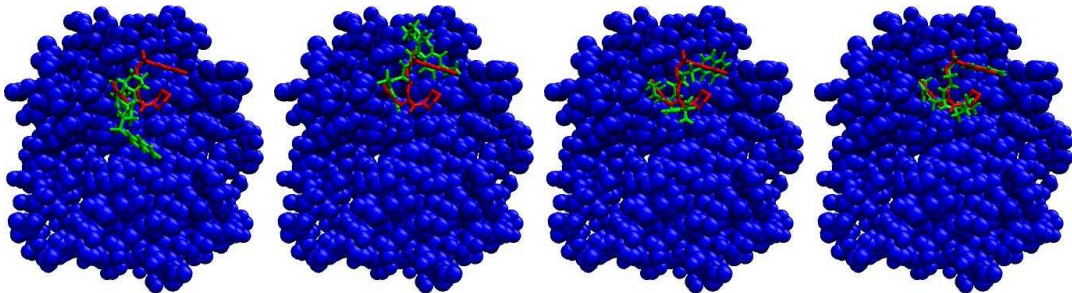
Prerequisites:

A solid algorithm background (graduate algorithm course CS5114) is required. No biology or chemistry knowledge is assumed (but interests in biological problems and a learning attitude are required). Interested students with life sciences background are welcome to disscuss with the instructor for the special permission (and possibly different requirements).

Class Information:

This class is intended for students who are interested in research in bioinformatics, in particular protein docking. There is no required textbook for this class. The class material will be mainly based on current research literature and a reference book: "Structural Bioinformatics" edited by Phil Bourne and Helge Weissig.

Grading will be based on (short) homework assignments (~30\%) and a long project (~70\%). Students can choose to do the project individually or as a group.