Structural Biochemistry (KBB056)

- Lecture on “Molecular surfaces and protein-protein docking”
- Graham Kemp (Computer Science and Engineering)
- http://www.cs.chalmers.se/~kemp/teaching/KBB056/

Aims

- To introduce alternative definintions of molecular surface.
- To describe alternative ways of representing molecular surfaces.
- To introduce the protein docking problem, and the Hex protein docking program.

Structural bioinformatics (TDA506)

In this course we consider "structural bioinformatics" to be the development and application of computational methods (i) to analyse and predict the conformations of biological macromolecules and (ii) to study relationships between macromolecular structure and function. Protein molecules will be in focus, but other biological molecules will also be studied.

Aims

- to present some of the computational challenges in structural biology;
- to describe computational methods for analysing and predicting macromolecular conformations and interactions; to give practice in programming techniques for structural bioinformatics.
- to give practice in the use of molecular graphics and modelling software;
- to emphasise the relationship between macromolecular shape and function.

Motivation

- Structural biology/biochemistry gives understanding of biological/biochemical function at the molecular level.
- These functions are ultimately due to interactions between molecules.
- Ideally, we want experimentally determined structures of molecules and complexes.
- Sometimes we have to rely on computer models of molecules and their interactions.

Structural bioinformatics (TDA506)

Content

three-dimensional structures of biological macromolecules; contact maps and distance maps; domain assignment; homogeneous transformation matrices; structure superposition; structure comparison; comparative protein modelling; protein fold recognition; Monte Carlo methods and simulated annealing; ab initio protein structure prediction; protein shape representation; protein-ligand interactions and applications in drug design; conformational analysis; protein-protein docking; modelling transmembrane proteins, carbohydrates and RNA; experimental protein structure determination using nuclear magnetic resonance (NMR) and X-ray crystallography; applications of structural bioinformatics.