Computational structural biology

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We develop and use computer modelling programs to determine biomolecular structures from sparse experimental data. The aim of our work is to understand the complex interactions between different molecules that form the basis of life and to address fundamental questions of molecular biology: What are the molecular structures of biologically important interactions? How do the involved molecules interact and how strong do they interact? How fast are these processes and what is the dynamical nature of the interacting components?

The computational structural biology group works closely with the experimental groups in biological chemistry, collaborators overseas, and performs structural mass spectrometry experiments within the group.

Projects for Summer 2012-2013

Modelling the structure of the E.coli DNA Replisome: a drug target. We have recently shown that very limited spatial restraints from paramagnetic NMR, chemical crosslinking or small angle light scattering experiments can be sufficient to determine the structure of protein complexes if the structures of the individual components are known. The individual structures of the 13 subunits of the E.coli DNA replisome have been solved by X-ray crystallography, however, the highly dynamic nature of the molecular machinery makes structural studies of the full complex difficult. The project will use bioinformatics to assemble the core complex with the help of sparse experimental data that was collected in our laboratory and by collaborators.

Probing intermolecular interactions in proteins. Intermolecular interactions are important in the regulation of vital cell processes and are key points for pharmaceutical intervention. This project will use flexible docking simulations to study the interaction of small peptides with a target protein using bioinformatically predicted contact sites and experimental NMR data.

More Information:
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