

## **Dr R Schmid - Bioinformatics and Molecular Modelling**

The wealth of sequence data in the postgenomics era provides us with the formidable challenge of thousands of novel proteins for which all we now is the sequence and the species the sequence is originating from. The major research interest of the group is to develop and apply computational methods to enhance our understanding of the structural, functional and evolutionary aspects of novel proteins. We develop and apply computational methods for structure prediction based on sequence such as fold recognition, threading and homology based structural modelling. To study functional aspect of individual proteins our methods of choice are ligand docking, protein-protein docking, electrostatic calculations and molecular dynamics. Protein targets are often chosen in collaboration with experimentally working colleagues. A further major interest of the group is in comparative genomics, in particular in the development of methods for high-throughput data analysis and automated functional annotation of sequence datasets. Examples for ongoing projects are:

- Improving protein-protein docking by implementing evolutionary and theoretically derived restraints
- Structure based inhibitor design for CDK-4
- Structure and function prediction for the ASP protein family
- dbESTmine and annot8r, bioinformatics resources for sequence annotation based on EST data

PhD projects are available in any of the mentioned research areas. Informal inquiries should be made by email to [rs206@le.ac.uk](mailto:rs206@le.ac.uk)