

Prediction of Protein Structures, Functions and Interactions

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The growing flood of new experimental data generated by genome sequencing has provided an impetus for the development of automated methods for predicting the functions of proteins that have been deduced by sequence analysis and lack experimental characterization.

Prediction of Protein Structures, Functions and Interactions presents a comprehensive overview of methods for prediction of protein structure or function, with the emphasis on their availability and possibilities for their combined use. Methods of modeling of individual proteins, prediction of their interactions, and docking of complexes are put in the context of predicting gene ontology (biological process, molecular function, and cellular component) and discussed in the light of their contribution to the emerging field of systems biology. Topics covered include:

- first steps of protein sequence analysis and structure prediction
- automated prediction of protein function from sequence
- template-based prediction of three-dimensional protein structures: fold-recognition and comparative modelling
- template-free prediction of three-dimensional protein structures
- quality assessment of protein models
- prediction of molecular interactions: from small ligands to large protein complexes
- macromolecular docking
- integrating prediction of structure, function, and interactions

Prediction of Protein Structures, Functions and Interactions focuses on the methods that have performed well in CASPs, and which are constantly developed and maintained, and are freely available to academic researchers either as web servers or programs for local installation. It is an essential guide to the newest, best methods for prediction of protein structure and functions, for researchers and advanced students working in structural bioinformatics, protein chemistry, structural biology and drug discovery.