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Biomolecular Modelling and Simulations

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The field of Biomolecular Modelling has evolved dramatically over the last ten years. The enormous growth in the computer power, construction of massive parallel super computers and the development of novel computational methods makes possible the successful simulation of increasingly large biomolecular systems. This thematic volume of APCSB includes review articles on advanced topics in biomolecular modelling and simulations such as: the interplay between molecular modelling and chemoinformatics, computational studies of DNA polymerase, dynamic modelling of molecular assembly, stability of amyloid oligomers, coarse-grained modelling of proteins, allosteric regulations in metal sensor proteins, modelling the N-acylethanolamine acid amidase inhibition and action, CHARMM-GUI online server for protein non-standard residues and high-resolution modelling of protein structures.

Cover image: Chemoinformatics and molecular modeling are complementary computational approaches for charting protein-ligand and protein-protein interactions landscapes. The two-dimensional plot shows a structure-activity similarity map generated with chemoinformatic methods for the systematic characterization of structure-activity relationships. The three-dimensional model illustrates a comparison of the binding modes of two small molecules with a therapeutic target. These models are essential tools for the structure-based design of drugs.

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