

PREFACE

Molecular modeling methods have received a fast growth over the last years due to the developments in CPU speed, the development of GPUs, the growth in high-performance computing capabilities, and new computational algorithms and theories. The applications of computational modeling methods in structural and chemical biology, and pharmaceutical chemistry also received a remarkable increase in integration with experimental, biochemical, structural, pharmaceutical, and spectroscopic studies. Nowadays, microsecond molecular dynamics simulations of large solvated protein-ligand complexes and membrane-based systems became available. The methods for dealing with the electronic structure of molecules and biomolecules became more accurate and applicable to larger systems. The combined quantum mechanics and molecular mechanics (QM/MM) methods received even broader applications to study enzymes and found novel implementations in drug design and chemical biology.

This volume of *Advances in Protein Chemistry and Structural Biology* is focused on some of the recent applications of computational modeling methods in the area of structural biology. In particular, one of the review chapters presents the state of the art of the QM/MM methods and their applications to study enzyme mechanisms and inhibition. Novel methods for efficient sampling of protein landscapes and disclosing allosteric regions are subject of another chapter. Further, the current state of the art of novel methods for design of inhibitors toward bromodomain BRD4 and QSAR models for knowledge discovery in databases is revealed. Finally, the modern computational methods for drug discovery of treatment of Chagas diseases are presented. Contributions from leading researchers in the field were selected to provide a good balance between the development of the computational methods and their implementations in the areas of structural biology, drug design, and enzymology.

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