

PREFACE

Enzymes play a crucial role in molecular processes in living organisms. They are characterized with the ability to increase considerably the rate of chemical reactions in the cells but also with high specificity toward their substrates. The key functions of enzymes in cell biology and unique properties make them important targets for drug design and applications in biotechnology, protein engineering, and synthetic biology.

Recent developments in experimental methods contribute for a rapid growth in our understanding about structure–function relationships in enzymes. Structural methods such as X-ray crystallography and NMR are currently widely used to determine the three-dimensional structures of enzymes, and their complexes with substrates and inhibitors. Homology modeling methods received growing applications to predict 3D structures of enzymes, when experimental structures are not available. In addition, spectroscopic and kinetic methods are broadly applied to complement structural information and understand enzyme structure–function relationships.

The applications of computational methods to enzyme mechanisms of functions received a large increase over the last years. The growth in computational power, the development of parallel supercomputers, and GPUs made possible modeling studies to be performed for very large biomolecular systems, containing hundreds of thousands of atoms. Nowadays, we can routinely perform molecular dynamics in order to understand the conformational flexibility of enzyme–ligand complexes in microsecond timescales, to apply combined quantum mechanical and molecular mechanical methods to explore the reaction mechanisms and the origins of the catalytic power in enzymes and to implement methods for prediction of the binding orientations and free energies of enzyme–ligand complexes.

The present thematic volume of *Advances in Protein Chemistry and Structural Biology* is aimed to address some of the recent developments in enzymes. The selected contributions are focused on state-of-the-art applications of computational and experimental methods to understand different aspects of structure–function relationships and mechanisms of enzymes and their applications in biotechnology, cell biology, drug design, and biomaterials.

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