
Preface

Over the years, molecular modeling and simulation of biomolecules has become an important tool in the molecular biosciences. Initially situated in the realm of specialists with in-depth knowledge of physics and computer science and access to supercomputers, molecular modeling is used increasingly by bioscientists who are mainly interested in investigating biological problems. This development has been supported by improved hardware, such as multi-core processors or graphic processing units, on the one hand, and accelerated sampling algorithms on the other hand that increase the timescale without increasing the demands on the hardware or the calculation time. The purpose of *Molecular Modeling of Proteins* is to provide a theoretical background of various methods available and to enable nonspecialists to apply methods to their problems. Most chapters contain, in addition to a thorough introduction, step-by-step instructions and notes on troubleshooting and how to avoid common pitfalls.

The current second edition of *Molecular Modeling of Proteins* provides some updated chapters and new material not covered in the first edition. The first part describes classical and advanced simulation methods as well as methods to set up complex systems such as lipid membranes and membrane proteins. The second part is devoted to the simulation and analysis of conformational changes of proteins, while Part III covers computational methods for protein structure prediction as well as using experimental data in combination with computational techniques. The final part contains chapters concerning protein–ligand interactions, which are relevant in the drug design process.

The topics cover some long established methods together with the latest developments in the field. The chapters are written by internationally renowned investigators: they include leading developers of popular simulation packages or force fields.

The second edition of *Molecular Modeling of Proteins* is directed at researchers in the physical-, chemical-, and biosciences working in industry and academia, who are interested in applying the methods in their own research. Additionally, the book forms a valuable resource for educators who wish to teach courses about molecular modeling.

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