

Preface

Although two decades ago molecular modeling and simulation of biomolecules were in the realm of specialists with access to supercomputers, ongoing improvements in force fields and powerful software readily available to the academic community have stimulated a great interest among bioscientists who are primarily interested in investigating biological or chemical problems. This development has been accompanied by a decrease in the price/performance ratio of hardware that enables us to carry out meaningful simulations on desktop workstations or small clusters of workstations. For example, all-atom models of a protein in a lipid membrane with water molecules included can be simulated for a few nanoseconds.

The purpose of *Molecular Modeling of Proteins* is to enable nonspecialists, first, to grasp the scope of methods available and, second, to apply methods easily to their own problems. Although software packages in molecular modeling are accompanied by good manuals, the first-time user may easily be frustrated over a problem that requires only a small tweak of an input file to solve. Thus, most chapters contain, apart from a thorough introduction, step-by-step instructions and notes on troubleshooting and hints about how to avoid pitfalls.

The first part of the book describes the methodologies of molecular modeling including a chapter about normal modes and essential dynamics. This part contains, apart from practical hints and tips, a thorough treatment of the underlying theories. The next part focuses on free energy calculations, followed by various chapters about the molecular modeling of membrane proteins. A later part contains chapters about protein structure determination by comparative protein modeling as well as modeling based on experimental data. A further part is devoted to the conformational changes of proteins, and protein folding and unfolding and misfolding in prion diseases. The last part contains several chapters about applications to drug design. The topics have been chosen to represent the latest developments in the field, albeit highly relevant to biochemical and biomedical problems. Although this book is directed at the modeling of proteins, the techniques described are equally applicable to other biomolecules, such as DNA or carbohydrates, provided the adequate force

fields are used. The chapters are written by internationally well-established investigators; they include leading developers of popular simulation packages or force fields.

Molecular Modeling of Proteins is directed to scientists in chemistry, biochemistry, biology, biophysics, and bioinformatics working in industry and academia, who are interested in applying the techniques described to their own research. Additionally, the book forms a valuable resource for educators who wish to teach courses to university students or professionals about molecular modeling.

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