Becker, O.M., McKerell, A.D., Jr., Roux, B., Watanabe, M.: **Computational Biochemistry and Biophysics.** – Marcel Dekker, New York – Basel 2001. ISBN 0-8247-0455-X. 512 pp., USD 195.00.

Molecular biochemistry and biophysics, and generally molecular biology, are strongly influenced by a fast development of the computational technique. This technique enables calculations of models which were not feasible in the past. This approach opens a very promising progress, from the solid fixed models of biomolecules to the dynamically moving objects. The motion (vibrations, rotations, fluctuations) is inherent to the molecular world. The study of molecular dynamics, a rapidly developing research field, is the main topic of the reviewed book. Basic objects of the study are proteins, nucleic acids, and biological membranes. 27 experts from all over the world took part in writing individual chapters of the book.

It is clear that the models are based on principal physical theories and approaches. The knowledge of mathematics and basic physical disciplines as are classical and statistical mechanics, thermodynamics, quantum mechanics, electrostatics, methods of quantum chemistry, *etc.*, may surely help to read the book easily. However, readers not fully acquainted with these theories will find basic introductions and relations and thus they may gain a deeper understanding of the problems. One goal of the book is to provide and explain deeper basics of the methods.

The book is divided into four parts. Each part is composed of several chapters. The chapters contain lists of references, some of them also a surveying conclusion and several examples. The reader will find very useful references for further more deep studies of the topics. It is not possible to mention here all the methods and questions dealt with in individual chapters. The content is very rich and comprehensive. I will mention only those most interesting for photosynthesis research.

The first part comprising 11 chapters concentrates on the basic computational methods. It explains the molecular dynamic simulations, fluctuations, and thermodynamics of motion. The approach is based on a combination of quantum, classical, and statistical mechanics. Because the problems are usually solved numerically, some computational algorithms are outlined. Among others, the concepts of genetic algorithms, conformational analysis, long-range forces and potentials, method of internal coordinates and energy minimisations, solvation effects, hydrophobic and electrostatic interactions, and normal mode analysis are treated. Methods studying reaction rates of enzymic processes, charge separation, and charge transfer are described.

Experimental methods revealing the molecular motion are described in two chapters of Part II. These are the liquid state nuclear magnetic resonance (NMR) and inelastic X-ray and neutron scattering. Part III concentrates on modelling of biological macromolecules (*e.g.*, the comparative modelling). Bayesian and frequent statistics suitable for the descriptions of complex biological models are explained in one chapter. Computer aided drug design is dealt with in the last chapter of this part.

Part IV deals with advanced applications, *e.g.*, with models and simulations of protein folding. The studies of electron transfer proteins, redox potential, or electron transfer rate calculations may be of special interest for researchers in photosynthesis and respiration. Mostly cytochromes and iron-sulfur proteins are accounted. The methods of simulating the nucleic acid molecules are surveyed. Last chapter deals with the simulations of structure and dynamics of biological membranes.

The Appendix at the end of the book and also some chapters contain references to the web sites with useful resources of the topic. The book is supplemented with a good subject index.

The book should be of interest for those working in molecular biological disciplines, and may serve both as a tool for the work and as a text-book for courses of dynamic and computational biochemistry and biophysics.

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