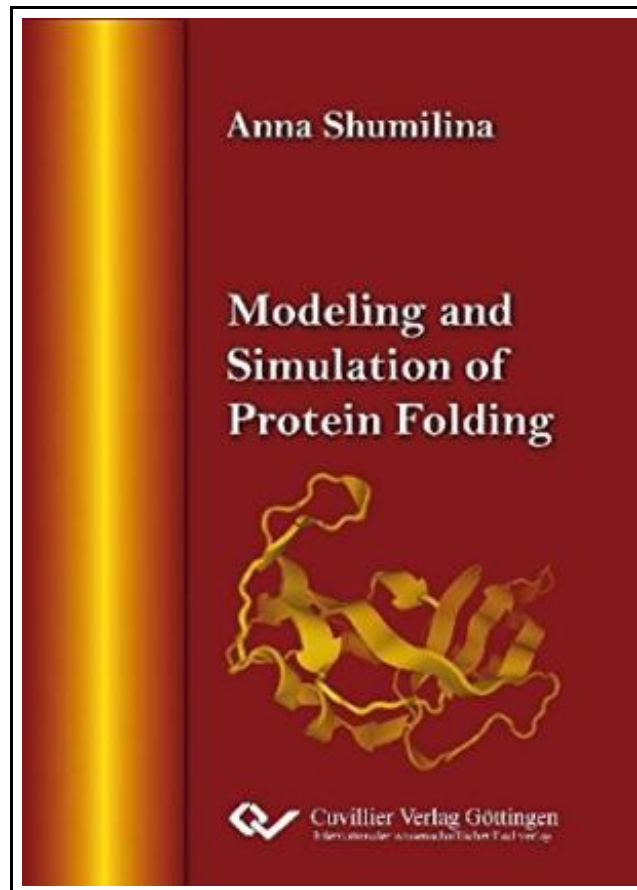# Modeling and Simulation of Protein Folding

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Reviews

Extensive manual! Its such a great read. It really is loaded with knowledge and wisdom You wont really feel monotony at at any time of your time (that's what catalogs are for regarding if you ask me).

(Myrl Hintz)

MODELING AND SIMULATION OF PROTEIN FOLDING

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Cuvillier Verlag Okt 2015, 2015. Taschenbuch. Book Condition: Neu. 211x149x17 mm. Neuware - The book describes a new mathematical model for intracellular protein folding and the implementation of this model in the form of a novel simulation software. Besides, the related biological, chemical, and physical background, important for understanding and rationalization of the proposed model, is outlined, and a short overview of the best-known methods for protein structure prediction and molecular modeling is given.The first chapter provides a general introduction to the problem, characterizes the chemical structure of proteins, and summarizes amino acid properties, including chirality and ionization behavior. After that, the principles of quantum mechanics and their consequences for the molecular structure are described. The discussion goes over to covalent and hydrogen bonding, as well as to electrostatic and van der Waals interactions. Further, some known facts about the three-dimensional structure of proteins and typical conformations of amino acids are outlined, followed by a quick glance at the hydrophobic effect and the interaction of charged groups with the solvent. Later on the focus is shifted to biological aspects, starting with chaperons and assisted protein folding, mentioning prions, which put into question the popular hypothesis about the global energy minimum of any native structure, and continuing with details of protein synthesis in the cell, which constituted the basis for the proposed model. The chapter finishes with a short description of experimental methods for protein structure prediction and with some information about databases for storage of known protein structures.The second chapter starts with a short overview of the knowledge-based protein structure prediction and ab initio protein folding approaches, then continues with empirical molecular mechanics force fields, typically used for molecular modeling. After that, it describes computation of atomic partial charges with a focus on the procedure of J. Gasteiger and M....

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