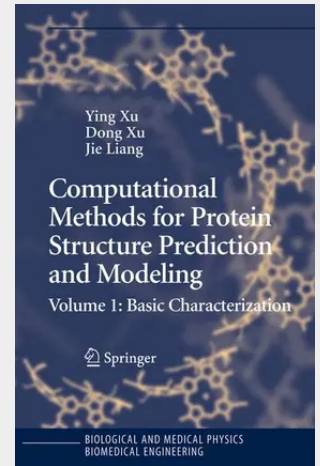


Computational Methods for Protein Structure Prediction and Modeling

Volume 1: Basic Characterization

An ultimate goal of modern biology is to understand how the genetic blueprint of cells (genotype) determines the structure, function, and behavior of a living organism (phenotype). At the center of this scientific endeavor is characterizing the biochemical and cellular roles of proteins, the working molecules of the machinery of life. A key to understanding of functional proteins is the knowledge of their folded structures in a cell, as the structures provide the basis for studying proteins' functions and functional mechanisms at the molecular level. Researchers working on structure determination have traditionally selected individual proteins due to their functional importance in a biological process or pathway of particular interest. Major research organizations often have their own protein X-ray crystallographic or/and nuclear magnetic resonance facilities for structure determination, which have been conducted at a rate of a few to dozens of structures a year. Realizing the widening gap between the rates of protein identification (through DNA sequencing and identification of potential genes through bioinformatics analysis) and the determination of protein structures, a number of large scientific initiatives have been launched in the past few years by government funding agencies in the United States, Europe, and Japan, with the intention to solve protein structures en masse, an effort called structural genomics. A number of structural genomics centers (factory-like facilities) have been established that promise to produce solved protein structures in a similar fashion to DNA sequencing.

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