

<<蛋白质计算机模拟>>

图书基本信息

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### 内容概要

This textbook covers a course of computer simulation of proteins for science major students , It consists of two knowledge blocks : Molecular Dynamics ( MD ) and Full Electron Structure Calculation of Proteins. We shall also discuss two main subjects: Knock-off Proteins and Protein-Lig and Interactions. However we shall not discuss the folding dynamics of proteins. These are discussed in "Cluster-Linux-Parallel Calculation System".

The Full Electron Structure Calculation of Proteins is one of the new features of this textbook. We assume the readers have the basic knowledge of computer languages , proteins and physics. Still , information on Unix , TCL and Phthon are included briefly in this textbook as a refreshing exercise. The keystone of this textbook is to elaborate the computer simulation of proteins. Therefore , merely reading this textbook is not enough. The students must practice all the problem examples on computers while studying. Otherwise , the students will not understand the topics discussed in this textbook.

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