PROTEIN COMPUTER SIMULATION

蛋白质计算机模拟

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-Ligand 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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