

Molecular Modeling and Simulation

An Interdisciplinary Guide

The basic goal of this new text is to introduce students to molecular modeling and simulation and to the wide range of biomolecular problems being attacked by computational techniques. The premise of the author is that the dazzling modeling and simulation software now available often leaves practitioners unaware of the fundamental problems and the complex algorithmic approaches to them that still form the heart of ongoing research. The text provides an overview of biomolecular modeling and structure, molecular mechanics (including functional construction and evaluation techniques), molecular graphics and visualization, techniques for conformational sampling (Monte Carlo, global optimization), methods for geometry optimization, and molecular dynamics simulations. Throughout the text emphasizes that the field changes very rapidly and that it is full of exciting discoveries, and that many of these findings lead to medical and technological breakthroughs. This book stimulates this excitement, while still providing students many computational details. The text evolved from Molecular Modeling courses taught by the author at New York University. It contains detailed illustrations throughout and homework assignments at the end of the book. It should appeal to beginning graduate students in medical schools, and in many scientific departments such as biology, chemistry, physics, mathematics and computer science.



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