



Computation of Biomolecular Structures Achievements, Problems, and Perspectives

By -

Springer. Paperback. Book Condition: New. Paperback. 223 pages. Dimensions: 9.0in. x 6.0in. x 0.6in. Computational techniques have become an indispensable part of Molecular Biology, Biochemistry, and Molecular Design. In conjunction with refined experimental methods and powerful hardware, they enable us to analyze and visualize biomolecular structures, simulate their motions and to a variable degree understand their physicochemical properties and function. In addition, they provide essentially the only way to analyze and correlate the astronomical amounts of experimental sequence and structural data accumulating in international databases. We have good reasons to believe that further advances in this area will eventually enable us to predict with sufficient accuracy many structural and functional properties of fairly large biomolecules, given their sequence and specified environmental conditions. However, it is also important to realize that in achieving this goal, we encounter several serious problems of conceptual and methodological nature, the solution of which requires new approaches and algorithms. For example, we need better force fields, more efficient optimization routines, an adequate description of electrostatics and hydration, reliable methods to compute free energies, and ways to extend the length of molecular dynamics simulations by several orders of magnitude. This item ships from multiple locations. Your book may...



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