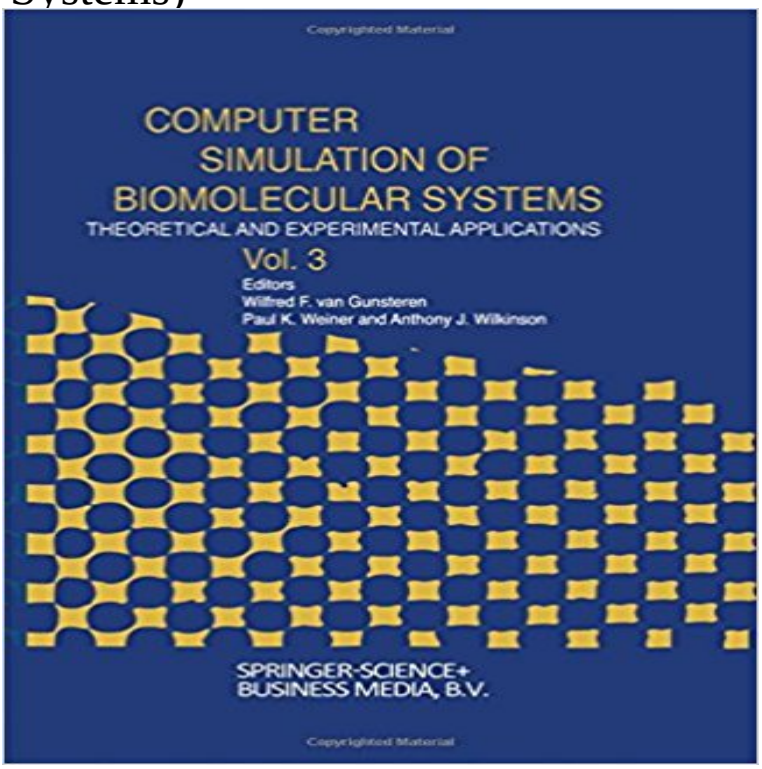
Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications (Computer Simulations of Biomolecular Systems)



The third volume in the series on Computer Simulation of Biomolecular Systems continues with the format introduced in the first volume [1] and elaborated in the second volume [2]. The primary emphasis is on the methodological aspects of simulations, although there are some chapters that present the results obtained for specific systems of biological interest. The focus of this volume has changed somewhat since there are several chapters devoted to structure-based ligand design, which had only a single chapter in the second volume. It seems useful to set the stage for this volume by quoting from my preface to Volume 2 [2]. The long-range goal of molecular approaches to biology is to describe living systems in terms of chemistry and physics. Over the last fifty years great progress has been made in applying the equations representing the underlying physical laws to chemical problems involv ing the structures and reactions of small molecules. Corresponding studies of mesoscopic systems have been undertaken much more recently. Molecular dynamics simulations, which are the primary focus of this volume, represent the most important theoretical approach to macromolecules of biological interest. ...

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(2000) Molecular dynamics and stochastic dynamics simulations, to appear in NATO ASI Series **Computer Simulation of Biomolecular Systems Theoretical and** Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications, Volume 3 contributions that highlight developments in methodology which enable longer and more realistic simulations (e.g. multiple time steps and **Computer Simulation of Biomolecular Systems - Google Books** Searching for Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications Volume 2 (Computer Simulations of Biomolecular **Computer Simulation of Biomolecular Systems: Theoretical and** Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications, Volume 1. Front Cover. Wilfred F. van Gunsteren, Paul K. Weiner. ESCOM, 1989 - Science Preface. 1. 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