Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology (Series in Computational Biophysics)

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Although molecular modeling has been around for a while, the groundbreaking advancement of massively parallel supercomputers and novel algorithms for parallelization is shaping this field into an exciting new area. Developments in molecular modeling from experimental and computational techniques have enabled a wide range of biological applications. Responding to this renaissance, **Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology** includes discussions of advanced techniques of molecular modeling and the latest research advancements in biomolecular applications from leading experts.

The book begins with a brief introduction of major methods and applications, then covers the development of cutting-edge methods/algorithms, new polarizable force fields, and massively parallel computing techniques, followed by descriptions of how these novel techniques can be applied in various research areas in molecular biology. It also examines the self-assembly of biomacromolecules, including protein folding, RNA folding, amyloid peptide aggregation, and membrane lipid bilayer formation. Additional topics highlight biomolecular interactions, including protein interactions with DNA/RNA, membrane, ligands, and nanoparticles. Discussion of emerging topics in biomolecular modeling such as DNA sequencing with solid-state nanopores and biological water under nanoconfinement round out the coverage.

This timely summary contains the perspectives of leading experts on this transformation in molecular biology and includes state-of-the-art examples of how molecular modeling approaches are being applied to critical questions in modern quantitative biology. It pulls together the latest research and applications of molecular modeling and real-world expertise that can boost your research and development of applications in this rapidly changing field.

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