



Biomolecules In Silico: Contemporary Advances in Computational Approaches to Investigating the Molecular Dynamics of Biological Systems

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Message from the Collection Editors

Dear Colleagues,

Molecular dynamics simulations allow us to investigate physically realistic behaviors of biological systems in exquisite spatial and temporal resolution. This information is utilized to elucidate an array of biophysical characteristics, such as stability in different conditions, relative propensity to adopt relevant conformations, discovery of transient binding pockets, etc. Molecular dynamics simulations are employed to garner a fundamental understanding of macromolecules that can be applied from basic science to drug discovery. In this Topical Collection, we report current advancements in algorithms, software, and analytical techniques that are related to molecular dynamics simulations of biological systems.

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Message from the Editorial Board

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