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

Collection Editors:

Dr. Thomas R. Caulfield
Department of Neuroscience, Division of QHS Computational Biology, Department of Artificial Intelligence and Informatics, Mayo Clinic, Jacksonville, FL 32224, USA

Dr. Manikandan Selvaraj
Department of Clinical Genomics, Mayo Clinic, Rochester, MN 55902, USA

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.

Dr. Thomas R. Caulfield
Dr. Manikandan Selvaraj
Collection Editors

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Message from the Editorial Board

Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

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Contact Us

Biomolecules Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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biomolecules@mdpi.com
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