Special Issue

Molecular Interactions and Advanced Computational Methods for Biomolecular Systems

Message from the Guest Editor

Molecular interactions are essential for the functionality of biomolecular systems, where proteins, nucleic acids, lipids, and other biomolecules engage in complex interactions that drive cellular processes such as protein folding, enzymatic activity, and gene regulation. These interactions are influenced by factors like hydrogen bonding, van der Waals forces, ionic interactions, and hydrophobic effects. Advanced computational methods are crucial for understanding how molecular crowding influences biomolecular systems. Techniques such as molecular dynamics (MD) simulations, Monte Carlo methods, and coarse-grained models allow for the study of biomolecular interactions.These models can inform drug design, particularly in optimizing the interaction of drug molecules with their targets in a crowded cellular environment. This Special Issue aims to highlight recent advancements in computational techniques and improved algorithms that have the potential to enhance our understanding of biomolecular systems and the effects of crowding on biological functions. These advancements are expected to provide new insights for therapeutic development and biomolecular engineering.

Guest Editor

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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