Special Issue

Deciphering Biomolecular Multimeric Systems: Computational Advances in Structure, Dynamics, and Function

Message from the Guest Editors

This Special Issue will showcase state-of-the-art computational approaches, including enhanced sampling techniques, machine learning-driven structural predictions, and integrative multi-scale modeling. By combining theoretical frameworks with experimental data, we seek to deepen our mechanistic understanding of biologically and pharmacologically relevant multimeric assemblies, such as membrane receptors, protein–protein complexes, PROTAC-mediated interactions, and molecular glue-stabilized formations. By fostering interdisciplinary synergies between computational modeling, biophysical experiments, and structural biology, we aspire to refine predictive models that accurately capture the conformational landscapes and cooperative interactions of these biomolecular systems. We particularly welcome contributions that address methodological advancements, develop novel theoretical frameworks, or provide mechanistic insights into multimeric complexes with implications for drug discovery, synthetic biology, and precision medicine. Through these collective efforts, we aim to accelerate the translation of fundamental discoveries into therapeutic and biotechnological innovations.

Guest Editors

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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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