

## Special Issue

# Structure, Molecular Dynamics, Assembly, and Evolution of Protein Systems with AI-Enhanced Modeling in Pharmacology and Structural Biology

### Message from the Guest Editors

Progress in protein biochemistry, molecular biology, pharmacology, and medicine cannot currently occur without an understanding of the structure, assembly, dynamics, and evolution of protein systems, as well as rational drug design. This Special Issue aims to highlight both experimental and computational advances in the characterization of protein folding, stability, assembly, and interactions – with a particular focus on protein–ligand systems and drug–target mechanisms. We welcome submissions on molecular dynamics simulations, protein evolution, structural bioinformatics, or ligand docking. Of particular interest are studies that integrate machine learning (ML) techniques with deep learning (DL) and Neural Networks (NNs) with cheminformatics to elucidate structure–function relationships, discover novel bioactive compounds, or model receptor-binding processes, including those for challenging protein classes. Appropriate experimental validation is essential for studies mainly relying on computational methods.

### Guest Editors

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### Deadline for manuscript submissions

closed (31 March 2026)



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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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