Special Issue

Computer Simulation Insight Into Ligand-Receptor Interaction

Message from the Guest Editor

Efforts to decipher the dynamic interplay between ligands and their molecular targets lies at the heart of drug discovery and design. This Special Issue invites cutting-edge contributions that leverage computational techniques to unravel binding mechanisms, guide hit-to-lead optimization, or enhance our understanding of receptor pharmacology.

We welcome original research, reviews, and perspectives covering state-of-the-art molecular dynamics applications, free energy calculation techniques, structure-based machine learning, and hybrid QM/MM, or physics-informed AI methods focusing on ligand–receptor interactions. Submissions addressing pharmaceutically relevant targets—such as GPCRs, enzymes, ion channels and protein–protein interfaces as well as RNA-binding small molecules—or integrating simulations with experimental and omics data are especially encouraged.

This Issue seeks to bridge disciplines and showcase innovations that push the boundaries of computational drug design and molecular recognition, accelerating translation from in silico prediction to therapeutic insight.

Guest Editor

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Deadline for manuscript submissions

30 April 2026

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/251181

International Journal of Molecular Sciences
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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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