

## Special Issue

# Advances in Protein–Ligand Interactions: From Structure, Function to Applications, 2nd Edition

### Message from the Guest Editor

Proteins function within a crowded cellular environment, interacting with various partners such as other proteins, small molecules, ions, and nucleic acids. Understanding these protein–ligand interactions (PLIs) is crucial for drug discovery. While experimental screening remains important, computational methods are increasingly valuable for efficiently narrowing down candidate compounds from large libraries.

This Special Issue seeks to highlight recent advances in PLI research, including but not limited to:

Protein surface analysis and binding site prediction

Molecular dynamics and de novo drug design

ADME studies, biochemical assays, and structural biology

Machine learning applications and clinical trial results

Theoretical models and open-source tools (with experimental validation)

We welcome both original research and review articles for consideration.

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### Guest Editor

Dr. Mateusz Banach

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### Deadline for manuscript submissions

30 June 2026



## Biomolecules

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**CiteScore 9.2**  
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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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