

Special Issue

Advances in Protein–Ligand Interactions

Message from the Guest Editor

Protein–ligand interactions are fundamental molecular phenomena in organisms. Proteins, which play important roles in various biological functions, depend on highly specific interactions with ligands to carry out their activities.

Protein–ligand interactions can exhibit remarkable specificity and efficiency, involving diverse types of ligands such as proteins, nucleic acids, lipids, small molecules, substrates, allosteric modulators, inhibitors, and drugs. These interactions play crucial roles in regulating signal transduction within cells, controlling metabolic pathways, facilitating physiological processes, and contributing to pathophysiological conditions. Therefore, comprehending the mechanisms underlying protein–ligand interactions, including their atomic-level binding modalities, conformational flexibility, and mutational effects, holds immense significance for drug design and advancements in biotechnology.

Contributions are invited that shed light on the importance of these interactions in biomedicine and molecular pathology, as well as their applications in biotechnology and the food industry.

Guest Editor

Prof. Dr. Dong-Jun Yu

School of Computer Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

Deadline for manuscript submissions

closed (20 July 2025)



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



mdpi.com/si/192784

*International Journal of
Molecular Sciences*
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

[mdpi.com/journal/
ijms](https://mdpi.com/journal/ijms)





International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



[mdpi.com/journal/
ijms](https://mdpi.com/journal/ijms)



About the Journal

Message from the Editor-in-Chief

The *International Journal of Molecular Sciences (IJMS)* 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, and molecular biophysics. *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.

Editor-in-Chief

Prof. Dr. José L. Quiles
Department of Physiology, Institute of Nutrition and Food Technology
"Jose Mataix", Biomedical Research Center, University of Granada,
Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)