

Special Issue

New Insights into Protein–Ligand Interactions

Message from the Guest Editor

Proteins, an important class of biological macromolecules, realize their functions through binding to themselves or other molecules. Protein–ligand interactions and multi-protein complexes perform central roles in the cellular systems of all living organisms, participating in their activation and regulation.

Protein interactions are also often at the basis of many pathological states. A detailed understanding of the protein–ligand interactions is therefore central to understanding biology at the molecular level and will also facilitate the discovery, design, and development of drugs, including (but not limited to) molecular docking, structure-based design, virtual screening of molecular fragments, small molecules and other types of compounds, clustering of complexes, and structural interpretation of activity cliffs, to name a few.

In this Special Issue of IJMS, we aim to collect contributions in the form of either original research articles or reviews, to add new insight into the role of protein–ligand interactions in biological processes and to highlight the state of the art, the challenges, and the open issues in this varied field of investigation.

Guest Editor

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Deadline for manuscript submissions

closed (31 May 2023)



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



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*International Journal of
Molecular Sciences*
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Message from the Editor-in-Chief

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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