

Special Issue

Recent Developments on Protein–Ligand Interactions: From Structure, Function to Applications 2.0

Message from the Guest Editor

Protein–ligand interactions play a fundamental role in most major biological functions, but also in drug discovery. With the increasing structural information of proteins and protein–ligand complexes, molecular modeling, molecular dynamics, and chemoinformatics approaches are often required for the efficient analysis of a large number of such complexes and to provide insights. Similarly, numerous computational approaches have been developed to characterize and use the knowledge of such interactions, which can lead to drug candidates. For instance, one main application is to identify tractable chemical start-points that non-covalently modulate the activity of a biological molecule. This new information brings questions that affect chemistry, biology, and even pose specific computer problems. Papers related to any aspect of protein–ligand analysis and/or prediction using computational approaches, as well as new developments dedicated to these tasks, will be considered for this Special Issue.

Guest Editor

Dr. Alexandre G. De Brevern

Department of Biological Research on the Red Blood Cells, INTS, INSERM UMR_S 1134, Université de Paris, Université de la Réunion, 75739 Paris, France

Deadline for manuscript submissions

closed (20 March 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/113070

*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*, 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.

Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle
Marche, Via Ranieri 65, 60100 Ancona, Italy

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, CAPlus / SciFinder, and other databases.

Journal Rank:

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