

## Special Issue

# Structure-Based Design of Drugs and Biologically Active Molecules Based on Computer-Aided Drug Discovery

### Message from the Guest Editor

Computer-Aided Drug Discovery (CADD) has advanced significantly, particularly with Structure-Based Drug Design (SBDD). SBDD uses three-dimensional models of biological targets, obtained by techniques such as X-ray crystallography and nuclear magnetic resonance (NMR), to guide the creation and optimization of bioactive molecules. SBDD allows the precise identification of ligands with high affinity and specificity, essential for therapeutic efficacy.

Computational tools, such as molecular docking and molecular dynamics, are employed to predict the conformation of ligands and their binding energies to the biological target. Molecular docking remains a vital tool in SBDD, allowing the prediction of the preferred orientation of a molecule in a protein target.

CADD and SBDD not only significantly reduce the time and cost associated with developing new drugs but also increase the accuracy in identifying promising compounds. The integration of computational and experimental methods is crucial for successful drug discovery, facilitating the identification and optimization of new drug candidates.

### Guest Editor

Dr. Cleudson Breno Rodrigues dos Santos  
Laboratory of Modeling and Computational Chemistry, Federal University of Amapá, Macapá 68902-280, Amapá, Brazil

### Deadline for manuscript submissions

20 March 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/209188](https://mdpi.com/si/209188)

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