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

**Deadline for manuscript submissions**

closed (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

*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

MDPI

# 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

MDPI

# 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, CAPlus / SciFinder, and other databases.

**Journal Rank:**

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