Special Issue

Computational Approaches in Drug Discovery and Design: From Molecular Modeling to Translational Applications

Message from the Guest Editor

This Special Issue aims to highlight recent advances in computational methods that are transforming modern drug discovery and development. Emphasis will be placed on the integration of molecular modeling, AI-driven drug design, molecular dynamics simulations, quantum chemical approaches, structure-based and ligand-based drug design, as well as multi-scale modeling in predicting pharmacokinetics, toxicity, and efficacy. Topics of interest include but are not limited to the following: in silico screening and optimisation of drug candidates; molecular docking and molecular dynamics simulations in target interaction studies; AI and machine learning in drug repurposing and de novo drug design; computational toxicology and safety prediction; pharmacophore modeling and virtual screening workflows; integration of omics data with modeling tools for personalised therapeutics; modeling of nanodrug behaviour and interactions at the cellular level; predictive models for ADME/T properties; and drug–drug interactions.

Guest Editor

Dr. Przemysław Czeleń

Department of Physical Chemistry, Faculty of Pharmacy, Collegium Medicum, Nicolaus Copernicus University, Kurpinskiego 5, 85-096 Bydgoszcz, Poland

Deadline for manuscript submissions

20 July 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/246353

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

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)