

Special Issue

Accelerating Therapeutic Innovation: Advances in Computer-Aided Drug Discovery

Message from the Guest Editors

This Special Issue on Computer-Aided Drug Discovery and Design (CADD) aims to present the latest advances and applications of computational methods in modern drug discovery, considering the continuous improvement of high-performance computing technologies. The goal of CADD methods is to improve and accelerate the drug discovery process. This issue will cover a wide range of CADD techniques, including traditional structure- and ligand-based drug design, possibly complemented by innovative machine learning approaches. We invite submissions that explore the application of CADD to address new challenges in drug discovery, such as the identification of novel therapeutic agents. Emphasis will be placed on innovative strategies that have undergone experimental (in vitro) validation, effectively linking computational predictions to practical outcomes.

Guest Editors

Dr. Pietro Delre

Department of Pharmacy, University of Naples Federico II, Via Domenico Montesano 49, 80131 Napoli, Italy

Prof. Dr. Antonio Lavecchia

Department of Pharmacy, "Drug Discovery Lab", University of Naples "Federico II", Via D. Montesano 49, 80131 Naples, Italy

Deadline for manuscript submissions

25 September 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/236594

*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)