

## Special Issue

# Advances in Computational Biology: Molecular Dynamics Simulation of Biomolecules

### Message from the Guest Editor

The simulation of important processes in biomedicine and biotechnology using computational methods has become a well-established field in recent years. We can simulate motions associated with the function of key macromolecules in cellular processes. Using molecular dynamics systems, we can study the effect of a mutation that causes a rare disease or a carcinogenic process on the structure and/or function of a macromolecule. We can also design molecules with the ability to act as antimicrobial, antiviral or anticancer agents. All these processes, as well as the methodology that makes them possible, are welcome in this Special Issue of *IJMS*.

### Guest Editor

Dr. Paulino Gómez-Puertas

Molecular Modeling Group, Centro de Biología Molecular Severo Ochoa (CBM, CSIC-UAM). CL Nicolas Cabrera, 1. Campus UAM, 28049 Madrid, Spain

### Deadline for manuscript submissions

20 August 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/209255](https://mdpi.com/si/209255)

*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)